HANDBOOK OF

Aqueous Solubility Data

SECOND EDITION

Samuel H. Yalkowsky
Yan He
Parijat Jain

CRC Press
Taylor & Francis Group

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Authors

Dr. Samuel Yalkowsky is professor of pharmaceutical sciences at the University of Arizona. He is currently involved in basic research on the relationships between chemical structure and physical phenomena such as solubility, partitioning, and melting. He has also made progress in the development of the state of the art algorithm for the estimation of the melting points, aqueous solubility and other physicochemical properties of organic compounds.

Dr. Yalkowsky is also involved in the alteration of solubility by physical means. This includes the development of formulations for insoluble drugs and the improved dissolution of environmentally important solutes from the soil. The formulation work was extended to include the development of novel dosage forms and the pharmaceutical evaluation of parenteral formulations. This has led to the development of novel methods for screening for hemolysis and for phlebitis.

Dr. Yan He earned her BS in biology from Wuhan University in 1992, her MS and PhD degrees in pharmaceutical sciences from the University of Arizona in 1999 and 2005. She is a senior research investigator in the Pharmaceuticals Sciences Department at Sanofi-Aventis. Her research interests include performing "drugability" assessment, providing formulation for preclinical studies, and preparing preformulation package for preclinical drug candidates. She also conducted basic research on the relationships between chemical structure and physical properties of organic compounds.

Dr. Parijat Jain received his PhD from the University of Arizona in 2008. Currently, he is a formulation scientist in the Pharmaceutical Development Unit at Novartis Pharmaceutical Corporation, East Hanover, NJ.

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Introduction

The *Handbook of Aqueous Solubility Data* is an extensive compilation of published data for the solubility of a very wide variety of organic nonelectrolytes and unionized weak electrolytes in water. It includes data for pharmaceuticals, pollutants, nutrients, herbicides, pesticides, agricultural, industrial, and energy-related compounds. This handbook contains over sixteen thousand solubility records for more than four thousand compounds. These data were extracted from about eighteen hundred scientific references, contained in the AQUASOL dATAbASE.

Each compound is identified by a sequential number with molecular formula, compound name, synonyms, molecular weight, Chemical Abstracts Service Registry Number, melting point, and boiling point if available. For user convenience, all solubility data are converted to moles per liter and grams per liter. Also, reported numerical temperature values are converted to centigrade. The following symbols are included in the temperature field when non-numerical temperature descriptors are reported:

amb	ambient temperature
c	cold water
h	hot water
rt	room temperature
ns	temperature not stated

Each record has a five-point evaluation for the reporting of the data and a reference code for the citation. Comments are included when necessary. The following alternatives are used in the comments field:

EFG	estimated from graph
LCST	lower critical solution temperature
UCST	upper critical solution temperature

Solubility Data

The compounds are sorted by their molecular formula using the Hill system (number of carbons, number of hydrogens, and then alphabetical by element), and then by name. Each compound can contain up to 5 synonyms. This is followed by the Chemical Abstracts Service Registry Number (RN), melting point (MP) in Celsius, molecular weight (MW), and boiling point (BP) in Celsius. Multiple values are presented whenever available. These are sorted by temperature and then by reference source.

Citations

The reference citation is given as a four-character code, in which the first character is alphabetic (referring to the first author's last name) and the next three are numeric. The complete reference citation is provided in the Reference section.

Evaluation

As listed in the Table of the Explanation of Evaluation Scores, a five-point evaluation is provided for the quality of the reporting of temperature (T), purity of solute (P), equilibration time/agitation (E), analysis (A), and accuracy and/or precision (A).

Explanation of Evaluation Scores

		Score		
Parameter		**0**	**1**	**2**
T	Temperature	Not given, ambient, or room temp	Given with no range	Given with range
P	Purity of solute	Not stated or as received	Stated with no range or as received	Stated with range or altered with range or calculated
E	Equilibration time/agitation	Not stated	Stated briefly	Described in detail
A	Analysis	Not stated	Stated briefly or stated in other paper	Described in detail
A	Accuracy and/or precision	1 significant figure or range > 20%	2 significant figures or range 5–20%	3 significant figures or range 1–5%

Indices

Entries in the indices are referenced to the sequential number, not to page numbers. The formulas in Index 3 are sorted by the Hill system.

Separate indices are provided for:

Index 1: Molecular Formula
Index 2: Names and Synonyms
Index 3: Chemical Abstracts Service Registry Number (RN)

Solubility Data

1. $CHBrCl_2$
Bromodichloromethane
Dichlorobromomethane
BDCM
RN: 75-27-4 **MP** (°C)**:** –55
MW: 163.83 **BP** (°C)**:** 87

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	3.032E+00	30	M300	1 1 2 2 2	
1.812E-02	2.968E+00	30	M311	1 1 2 2 2	

2. $CHBr_2Cl$
Chlorodibromomethane
Dibromochloromethane
CDBM
RN: 124-48-1 **MP** (°C)**:** –22
MW: 208.29 **BP** (°C)**:** 119.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E-03	1.050E+00	30	M300	1 1 2 2 2	
1.205E-02	2.509E+00	30	M311	1 1 2 2 2	

3. $CHBr_3$
Bromoform
Tribromomethane
Methyl tribromide
RN: 75-25-2 **MP** (°C)**:** 7.5
MW: 252.75 BP (°C)**:** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	3.001E+00	15	G029	1 0 2 2 2	
3.957E-03	1.000E+00	20	F300	1 0 0 0 0	
<7.91E-04	<2.00E-01	25	B019	1 0 1 2 0	*sic*
1.262E-02	3.190E+00	30	F300	1 0 0 0 2	
1.258E-02	3.180E+00	30	G029	1 0 2 2 2	
1.555E-02	3.931E+00	30	M311	1 1 2 2 2	
1.256E-02	3.174E+00	30	V009	1 0 0 0 2	
1.227E-02	3.100E+00	ns	O006	0 0 0 0 2	

4. $CHClF_2$
Chlorodifluoromethane
Freon 22
Halocarbon 22
RN: 75-45-6 **MP** (°C)**:** –146
MW: 86.47 **BP** (°C)**:** –40.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.018E-01	2.610E+01	21	M065	1 0 2 1 2	

5. $CHCl_3$
Chloroform
Trichloromethane
Methyl trichloride
Formyl trichloride
RN: 67-66-3 **MP** (°C)**:** –63
MW: 119.38 **BP** (°C)**:** 61

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-02	1.062E+01	0	H101	2 0 0 0 2	
7.077E-02	8.448E+00	15	G029	1 0 2 2 2	
7.134E-02	8.517E+00	15	J036	0 0 0 0 0	
6.648E-02	7.937E+00	20	E019	1 0 1 1 0	
6.785E-02	8.100E+00	20	F300	1 0 0 0 1	
6.886E-02	8.220E+00	20	H101	2 0 0 0 2	
6.869E-02	8.200E+00	20	M133	1 0 0 0 2	
6.827E-02	8.150E+00	20	M368	1 0 0 0 1	
6.648E-02	7.937E+00	20	N034	1 0 0 0 0	
6.869E-02	8.200E+00	20	P046	1 0 0 0 0	
6.750E-02	8.058E+00	20	P073	1 0 0 1 2	
3.504E-02	4.182E+00	22	H072	1 0 1 1 2	
7.472E-02	8.920E+00	25	B019	1 0 1 2 0	
6.050E-02	7.222E+00	25	B173	2 0 2 2 2	
6.660E-02	7.950E+00	25	F071	1 1 2 1 2	
6.648E-02	7.937E+00	25	G056	1 0 0 0 2	
6.813E-02	8.133E+00	25	L319	1 0 2 1 2	
6.618E-02	7.900E+00	25	M037	1 1 0 0 1	
6.648E-02	7.937E+00	25	O026	1 2 0 1 0	
7.472E-02	8.920E+00	25	R321	1 2 1 1 1	
6.236E-02	7.444E+00	25.0	C055	1 2 1 0 1	
6.409E-02	7.651E+00	30	G029	1 0 2 2 2	
6.500E-02	7.760E+00	30	H101	2 0 0 0 2	
2.114E-02	2.524E+00	30	M311	1 1 2 2 2	
6.411E-02	7.653E+00	30	V009	1 0 0 0 2	
6.648E-02	7.937E+00	56.1	C055	2 2 1 0 0	
6.236E-02	7.444E+00	60	R321	1 2 1 1 1	
6.660E-02	7.950E+00	ns	H123	0 0 0 0 0	

(*continued*)

5. $CHCl_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.168E-02	4.975E+00	ns	I306	0 0 0 0 0	
6.660E-02	7.950E+00	ns	M344	0 0 0 0 2	
6.830E-02	8.153E+00	ns	R028	0 0 0 0 0	

6. CHI_3

Iodoform
Triiodomethane

RN: 75-47-8 **MP** (°C)**:** 121.5
MW: 393.73 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	1.181E-01	25	V009	1 0 0 0 0	
2.540E-04	9.999E-02	rt	D021	0 0 1 1 0	

7. CH_2BrCl

Bromochloromethane
Bromo-chloro-methane
Chlorobromomethane
CBM

RN: 74-97-5 **MP** (°C)**:** –86.5
MW: 129.39 **BP** (°C)**:** 68.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-01	1.669E+01	25	M342	1 0 1 1 2	
1.142E-01	1.478E+01	ns	O006	0 0 0 0 1	

8. CH_2Br_2

Methylene bromide
Dibrom-methan

RN: 74-95-3 **MP** (°C)**:** –52.7
MW: 173.85 **BP** (°C)**:** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-02	1.173E+01	0	H101	2 0 0 0 2	
6.652E-02	1.156E+01	15	G029	1 0 2 2 2	
6.604E-02	1.148E+01	20	H101	2 0 0 0 2	
6.259E-02	1.088E+01	25	O006	1 0 0 0 1	
6.782E-02	1.179E+01	30	G029	1 0 2 2 2	

(*continued*)

8. CH_2Br_2 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.765E-02	1.176E+01	30	H101	2 0 0 0 2	
6.779E-02	1.179E+01	30	V009	1 0 0 0 2	
6.558E-02	1.140E+01	ns	F300	0 0 0 0 2	

9. CH_2Cl_2

Methylene chloride
Dichlor-methan
Dichloromethane
Methylene dichloride
Methane dichloride

RN: 75-09-2 **MP** (°C)**:** –95.1
MW: 84.93 **BP** (°C)**:** 39.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.782E-01	2.363E+01	0	H101	2 0 0 0 2	
2.309E-01	1.961E+01	20	C057	0 0 0 0 0	
2.355E-01	2.000E+01	20	F300	1 0 0 0 0	
2.355E-01	2.000E+01	20	H101	2 0 0 0 2	
2.263E-01	1.922E+01	20	N034	1 0 0 0 2	
1.887E-01	1.603E+01	20	N038	1 0 0 1 2	
2.309E-01	1.961E+01	25	A094	1 0 0 0 1	
1.534E-01	1.303E+01	25	G056	1 0 0 0 2	
1.554E-01	1.320E+01	25	M037	1 1 0 0 2	
1.554E-01	1.320E+01	25	M133	1 0 0 0 2	
1.554E-01	1.320E+01	25	P046	1 0 0 0 0	
2.275E-01	1.932E+01	30	V009	1 0 0 0 2	
2.284E-01	1.940E+01	ns	H123	0 0 0 0 0	

10. CH_2I_2

Methylene iodide
Diiod-methan

RN: 75-11-6 **MP** (°C)**:** 6.0
MW: 267.84 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-03	8.330E-01	25	A032	1 2 1 1 2	
4.624E-03	1.238E+00	30	G029	1 0 2 2 2	
4.594E-03	1.231E+00	30	V009	1 0 0 0 1	

11. CH_2N_2
Cyanamide
Cyanamid
RN: 420-04-2 **MP** (°C)**:**
MW: 42.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E+01	4.444E+02	ns	N013	0 0 0 0 1	

12. CH_3Br
Methyl bromide
Bromomethane
Celfume
RN: 74-83-9 **MP** (°C)**:** –94
MW: 94.94 **BP** (°C)**:** 3.56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-01	2.609E+01	10	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	M061	1 0 0 0 2	
1.933E-01	1.835E+01	19.9	G061	1 2 1 1 2	774.3mm Hg @ 25 °C
1.685E-01	1.600E+01	20	G080	1 0 0 0 1	
1.659E-01	1.575E+01	20	P081	1 0 0 0 1	
1.394E-01	1.323E+01	25	H081	1 0 2 0 2	
1.411E-01	1.340E+01	25	M161	1 0 0 0 2	
1.196E-01	1.136E+01	32	H081	1 0 2 0 2	
9.479E-03	9.000E-01	ns	N013	0 0 0 0 1	

13. $CH_3BrO_6S_2$
Bromomethionic acid
Methanedisulfonic acid, bromo-
RN: 187610-86-2 **MP** (°C)**:**
MW: 255.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.039E+00	7.752E+02	25	B077	1 2 0 0 2	

14. CH_3Cl

Methyl chloride
Chloromethane

RN: 74-87-3 **MP** (°C)**:** –97.0
MW: 50.49 **BP** (°C)**:** –23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+01	7.727E+02	0	M061	1 0 0 0 1	*sic*
1.436E-01	7.250E+00	20	M133	1 0 0 0 2	
9.069E-02	4.579E+00	20	N034	1 0 0 0 1	
1.436E-01	7.250E+00	20	P046	1 0 0 0 0	
1.059E-01	5.347E+00	24.9	G061	1 2 1 1 2	756.1mm Hg @ 25 °C
1.455E-01	7.346E+00	30	G056	1 0 0 0 2	
1.466E-01	7.400E+00	30	M037	1 1 0 0 1	

15. $CH_3ClO_6S_2$

Chloromethionic acid
Acide chloromethionique

RN: 74692-14-1 **MP** (°C)**:**
MW: 210.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.540E+01	3.243E+03	25	B075	1 2 0 0 2	

16. CH_3F

Fluoromethane
Methylfluoride

RN: 593-53-3 **MP** (°C)**:** –141.8
MW: 34.03 **BP** (°C)**:** –78.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~7.05E-02	~2.40E+00	15	F300	1 0 0 0 0	
5.250E-02	1.787E+00	29.9	G061	1 2 1 1 2	766.8mm Hg @25 °C

17. CH_3I
Iodomethane
Methyl-iodide
Halon 10001
Methyl iodine
Methyliodide
RN: 74-88-4 **MP** (°C)**:** –64
MW: 141.94 **BP** (°C)**:** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-01	1.565E+01	0	H101	2 0 0 0 2	
9.997E-02	1.419E+01	20	H101	2 0 0 0 2	
9.727E-02	1.381E+01	20	H127	1 0 0 0 1	
9.727E-02	1.381E+01	20	I316	0 0 0 0 0	
9.600E-02	1.363E+01	20	M171	1 0 0 0 2	
9.590E-02	1.361E+01	22	F001	1 0 1 2 2	
9.511E-02	1.350E+01	22	F300	1 0 0 0 2	
9.590E-02	1.361E+01	22	S006	1 0 0 0 2	
1.007E-01	1.429E+01	30	H101	2 0 0 0 2	
9.957E-02	1.413E+01	30	V009	1 0 0 0 2	
8.725E-03	1.238E+00	ns	O006	0 0 0 0 1	

18. CH_3NO
Formaldehyde oxime
Formaldehyd-oxim
RN: 75-17-2 **MP** (°C)**:**
MW: 45.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.774E+00	1.700E+02	20	F300	1 0 0 0 1	

19. CH_3NO_2
Nitromethane
Nitrocarbol
NM
RN: 75-52-5 **MP** (°C)**:** –29
MW: 61.04 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E+00	8.676E+01	20	C121	0 0 0 0 1	unit assumed, *sic*
1.627E+00	9.934E+01	25	F049	2 0 2 0 0	
1.802E+00	1.100E+02	25	M136	2 0 0 0 2	
1.802E+00	1.100E+02	25	M139	2 0 0 0 2	
3.039E-01	1.855E+01	ns	D348	0 0 0 0 0	

20. CH_3N_5
5-Aminotetrazole
5-Amino-tetrazol
RN: 4418-61-5 **MP** (°C)**:** 204
MW: 85.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.411E-01	1.200E+01	18	F300	1 0 0 0 1	

21. CH_4
Methane
Methan
RN: 74-82-8 **MP** (°C)**:** –183
MW: 16.04 **BP** (°C)**:** –161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.468E-03	3.960E-02	0	F300	1 0 0 0 2	
2.210E-03	3.545E-02	4.99	C115	2 0 2 2 2	
1.926E-03	3.090E-02	9.99	C115	2 0 2 2 2	
1.633E-03	2.620E-02	14.99	C115	2 0 2 2 2	
1.567E-03	2.513E-02	19.8	G058	1 0 0 0 2	
1.511E-03	2.424E-02	19.99	C115	2 0 2 2 2	
1.446E-03	2.320E-02	20	F300	1 0 0 0 2	
1.381E-03	2.215E-02	24.99	C115	2 0 2 2 2	
1.521E-03	2.440E-02	25	M001	2 1 2 2 2	
1.521E-03	2.440E-02	25	M002	2 2 1 2 2	
1.502E-03	2.410E-02	25	M040	1 0 0 1 2	
1.550E-03	2.487E-02	25	M102	1 2 2 1 2	
1.266E-03	2.030E-02	29.99	C115	2 0 2 2 2	
1.189E-03	1.907E-02	34.99	C115	2 0 2 2 2	
1.079E-03	1.732E-02	39.99	C115	2 0 2 2 2	
1.056E-03	1.693E-02	40	S212	2 1 2 2 2	
1.055E-03	1.693E-02	44.99	C115	2 0 2 2 2	
8.477E-04	1.360E-02	50	F300	1 0 0 0 2	
9.000E-04	1.444E-02	60	S212	2 1 2 2 2	
8.000E-04	1.283E-02	80	S212	2 1 2 2 2	
1.434E-03	2.300E-02	ns	M091	0 1 0 0 2	
1.378E-03	2.210E-02	ns	S212	2 1 2 2 2	

22. CH_4N_2O

Urea
Harnstoff
Uree

RN: 57-13-6 **MP** (°C)**:** 132.7
MW: 60.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E+00	4.012E+02	0	F300	1 0 0 0 2	
4.757E+00	2.857E+02	0	J021	1 0 0 0 2	
6.680E+00	4.012E+02	0	M043	1 0 0 0 1	
6.680E+00	4.012E+02	0	P023	1 2 1 1 2	
7.297E+00	4.382E+02	5	D041	1 0 0 0 1	
5.088E+00	3.056E+02	7	J021	1 0 0 0 2	
5.246E+00	3.151E+02	10	D020	1 2 1 1 2	
5.246E+00	3.151E+02	10	D060	2 2 1 1 2	
7.651E+00	4.595E+02	10	M043	1 0 0 0 1	
7.602E+00	4.565E+02	10	P023	1 2 1 1 2	
5.550E+00	3.333E+02	17	J021	1 0 0 0 2	
7.382E+00	4.433E+02	18.72	S131	2 2 1 1 2	recrystallized
5.536E+00	3.324E+02	20	C052	1 2 1 1 2	
5.617E+00	3.373E+02	20	J021	1 0 0 0 2	
8.529E+00	5.122E+02	20	M043	1 0 0 0 2	
8.517E+00	5.115E+02	20	P023	1 2 1 1 2	
7.594E+00	4.561E+02	21.59	S131	2 2 1 1 2	recrystallized
7.738E+00	4.647E+02	23.85	S131	2 2 1 1 2	recrystallized
5.874E+00	3.528E+02	25	D020	1 2 1 1 2	
9.058E+00	5.440E+02	25	D041	1 0 0 0 2	
5.874E+00	3.528E+02	25	D060	2 2 1 1 2	
8.326E+00	5.000E+02	25	M136	2 0 0 0 2	
7.910E+00	4.750E+02	26.83	S131	2 2 1 1 2	recrystallized
7.966E+00	4.784E+02	27.31	S131	2 2 1 1 2	recrystallized
9.566E+00	5.745E+02	30	M043	1 0 0 0 2	
9.596E+00	5.763E+02	30	P023	1 2 1 1 2	
8.171E+00	4.907E+02	30.38	S131	2 2 1 1 2	recrystallized
6.244E+00	3.750E+02	35	J021	1 0 0 0 2	
1.712E+01	1.028E+03	35	S200	1 0 0 0 2	loc. cit.
8.469E+00	5.086E+02	35.15	S131	2 2 1 1 2	recrystallized
8.465E+00	5.083E+02	35.42	S131	2 2 1 1 2	recrystallized
8.575E+00	5.150E+02	37.36	S131	2 2 1 1 2	recrystallized
1.038E+01	6.232E+02	39.7	P023	1 2 1 1 2	
6.392E+00	3.839E+02	40	D020	1 2 1 1 2	
6.392E+00	3.839E+02	40	D060	2 2 1 1 2	
1.037E+01	6.226E+02	40	M043	1 0 0 0 2	
1.837E+01	1.103E+03	40	S200	1 0 0 0 2	loc. cit.
8.822E+00	5.298E+02	41.11	S131	2 2 1 1 2	recrystallized
8.982E+00	5.394E+02	43.85	S131	2 2 1 1 2	recrystallized
8.967E+00	5.386E+02	43.94	S131	2 2 1 1 2	recrystallized
1.961E+01	1.178E+03	45	S200	1 0 0 0 2	loc. cit.
9.107E+00	5.469E+02	46.56	S131	2 2 1 1 2	recrystallized
1.119E+01	6.721E+02	50	P023	1 2 1 1 2	

(*continued*)

22. CH_4N_2O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+01	1.267E+03	50	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.736E+02	50.6	P023	1 2 1 1 2	
9.560E+00	5.742E+02	54.77	S131	2 2 1 1 2	recrystallized
9.584E+00	5.756E+02	54.97	S131	2 2 1 1 2	recrystallized
2.283E+01	1.371E+03	55	S200	1 0 0 0 2	loc. cit.
9.649E+00	5.795E+02	55.88	S131	2 2 1 1 2	recrystallized
9.681E+00	5.814E+02	57.02	S131	2 2 1 1 2	recrystallized
9.806E+00	5.889E+02	59.13	S131	2 2 1 1 2	recrystallized
6.936E+00	4.166E+02	60	J021	1 0 0 0 2	
9.847E+00	5.914E+02	60	K013	1 0 1 1 2	
1.189E+01	7.143E+02	60	M043	1 0 0 0 2	
2.422E+01	1.455E+03	60	S200	1 0 0 0 2	loc. cit.
1.184E+01	7.110E+02	60.0	P023	1 2 1 1 2	
9.930E+00	5.963E+02	61.76	S131	2 2 1 1 2	recrystallized
1.005E+01	6.034E+02	63.79	S131	2 2 1 1 2	recrystallized
1.009E+01	6.060E+02	65	K013	1 0 1 1 2	
2.570E+01	1.543E+03	65	S200	1 0 0 0 2	loc. cit.
1.244E+01	7.468E+02	68.5	P023	1 2 1 1 2	
1.020E+01	6.127E+02	68.50	M059	1 1 2 1 2	
1.270E+01	7.629E+02	70	F300	1 0 0 0 2	
7.206E+00	4.328E+02	70	J021	1 0 0 0 2	
1.033E+01	6.206E+02	70	K013	1 0 1 1 2	
1.263E+01	7.588E+02	70	P023	1 2 1 1 2	
2.730E+01	1.640E+03	70	S200	1 0 0 0 2	loc. cit.
1.038E+01	6.231E+02	70.49	S131	2 2 1 1 2	recrystallized
1.048E+01	6.295E+02	73.11	S131	2 2 1 1 2	recrystallized
1.057E+01	6.345E+02	75	K013	1 0 1 1 2	
1.048E+01	6.296E+02	75.30	M059	1 1 2 1 2	
1.079E+01	6.480E+02	80	K013	1 0 1 1 2	
1.332E+01	8.000E+02	80	M043	1 0 0 0 2	
1.090E+01	6.546E+02	84.40	M059	1 1 2 1 2	
1.101E+01	6.610E+02	85	K013	1 0 1 1 2	
3.229E+01	1.939E+03	85	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.738E+02	90	K013	1 0 1 1 2	
3.426E+01	2.058E+03	90	S200	1 0 0 0 2	loc. cit.
1.131E+01	6.791E+02	93.80	M059	1 1 2 1 2	
1.142E+01	6.858E+02	95	K013	1 0 1 1 2	
3.611E+01	2.169E+03	95	S200	1 0 0 0 2	loc. cit.
1.161E+01	6.975E+02	100	K013	1 0 1 1 2	
1.465E+01	8.795E+02	100	M043	1 0 0 0 2	
3.778E+01	2.269E+03	100	S200	1 0 0 0 2	loc. cit.
1.177E+01	7.066E+02	104.40	M059	1 1 2 1 2	
1.199E+01	7.199E+02	109.90	M059	1 1 2 1 2	
1.219E+01	7.321E+02	115.30	M059	1 1 2 1 2	
1.229E+01	7.383E+02	118.30	M059	1 1 2 1 2	
1.234E+01	7.411E+02	118.70	M059	1 1 2 1 2	
1.245E+01	7.479E+02	121.90	M059	1 1 2 1 2	
1.249E+01	7.503E+02	123.20	M059	1 1 2 1 2	
1.264E+01	7.592E+02	127.50	M059	1 1 2 1 2	

(*continued*)

22. CH_4N_2O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E+01	7.619E+02	128.80	M059	1 1 2 1 2	
1.281E+01	7.694E+02	132.60	M059	1 1 2 1 2	
1.665E+01	1.000E+03	ns	B338	0 0 0 0 1	
1.332E+01	8.000E+02	ns	D072	0 0 0 0 0	

23. CH_4N_2S

Thiourea
Thiouree

RN: 62-56-6 **MP** (°C)**:** 176
MW: 76.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.136E-01	4.671E+01	0	M043	1 0 0 0 1	
9.731E-01	7.407E+01	10	M043	1 0 0 0 1	
1.118E+00	8.507E+01	10	O017	1 0 1 1 2	
1.206E+00	9.180E+01	13	F300	1 0 0 0 2	
1.206E+00	9.179E+01	13	O019	1 0 0 1 2	
1.383E+00	1.053E+02	15	O017	1 0 1 1 2	
1.573E+00	1.197E+02	20	M043	1 0 0 0 2	
1.544E+00	1.175E+02	20	O017	1 0 1 1 2	
1.085E+00	8.257E+01	25	I310	0 0 0 0 0	
1.759E+00	1.339E+02	25	O017	1 0 1 1 2	
2.199E+00	1.674E+02	30	M043	1 0 0 0 2	
3.093E+00	2.355E+02	40	M043	1 0 0 0 2	
5.455E+00	4.152E+02	60	M043	1 0 0 0 1	
7.617E+00	5.798E+02	80	M043	1 0 0 0 2	
9.250E+00	7.041E+02	100	M043	1 0 0 0 2	
7.882E-01	6.000E+01	ns	D072	0 0 0 0 0	

24. $CH_4N_4O_2$

α-Nitroguanidine
Nitroguanidine
Nitroguanidin

RN: 556-88-7 **MP** (°C)**:** 235
MW: 104.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.597E-02	2.703E+00	19.5	D027	1 2 0 0 2	
1.173E-01	1.221E+01	25	D022	1 1 2 2 2	
4.228E-02	4.400E+00	25	F300	1 0 0 0 1	
4.305E-02	4.480E+00	29.87	M028	1 2 2 1 0	EFG
1.122E-01	1.167E+01	50	D027	1 2 0 0 2	
3.070E-01	3.195E+01	71.67	M028	1 2 2 1 0	EFG
5.695E-01	5.927E+01	83.98	M028	1 2 2 1 0	EFG
9.025E-01	9.392E+01	100	D027	1 2 0 0 2	
7.620E-01	7.930E+01	100	F300	1 0 0 0 2	

25. CH_4O
Methanol
Methyl alcohol
RN: 67-56-1 **MP** (°C)**:** –97.8
MW: 32.04 **BP** (°C)**:** 64.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E+01	5.411E+02	ns	L003	0 0 2 1 2	

26. $CH_4O_6S_2$
Methionic acid
Acide methionique
Methanedisulfonic acid
RN: 503-40-2 **MP** (°C)**:** 98.0
MW: 176.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E+01	2.458E+03	25	B075	1 2 0 0 2	
4.035E+00	7.108E+02	25	B076	1 2 0 0 2	
4.862E+00	8.566E+02	25	F300	1 0 0 0 2	

27. $CH_4O_6S_2.H_2O$
Methionic acid (monohydrate)
RN: 503-40-2 MP (°C)**:**
MW: 194.18 BP (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.409E+00	8.562E+02	25	B076	1 2 0 0 2	

28. CH_5N
Methylamine
Aminomethane
Carbinamine
Mercurialin
RN: 74-89-5 **MP** (°C)**:** –93.5
MW: 31.06 **BP** (°C)**:** –6.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.906E+01	5.920E+02	4.50	F300	1 0 0 0 2	
2.963E+01	9.202E+02	12.5	D041	1 0 0 0 2	
2.147E+01	6.667E+02	12.50	M081	1 0 0 0 2	
1.916E+01	5.951E+02	20	M081	1 0 0 0 2	

(*continued*)

28. CH_5N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E+01	5.556E+02	25	M081	1 0 0 0 2	
1.664E+01	5.169E+02	30	M081	1 0 0 0 2	
1.380E+01	4.286E+02	40	M081	1 0 0 0 1	
1.143E+01	3.548E+02	50	M081	1 0 0 0 1	
9.034E+00	2.806E+02	60	M081	1 0 0 0 1	

29. $CH_5N_5O_2$
Nitroaminoguanidine
Hydrazinecarboximidamide, *N*-nitro-
1-Amino-3-nitroguanidine
3-Amino-1-nitroguanidine
1-Amino-2-nitroguanidine
1-Nitro-3-aminoguanidine
RN: 18264-75-0 **MP** (°C)**:** 185
MW: 119.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	1.619E+00	9.33	M047	2 2 1 1 0	EFG
2.254E-02	2.684E+00	20.96	M047	2 2 1 1 0	EFG
3.567E-02	4.248E+00	29.87	M047	2 2 1 1 0	EFG
4.384E-02	5.221E+00	34.53	M047	2 2 1 1 0	EFG
7.087E-02	8.440E+00	44.30	M047	2 2 1 1 0	EFG
9.318E-02	1.110E+01	49.42	M047	2 2 1 1 0	EFG

30. CH_5O_3As
Methanearsonic acid
MAA
Methylarsonsaeure
RN: 124-58-3 **MP** (°C)**:** 132
MW: 139.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E+00	2.038E+02	20	B200	1 0 0 0 2	
1.563E+00	2.188E+02	25	D305	1 0 0 0 1	

31. CH_5As
Methylarsine
Methylarsin
RN: 593-52-2 **MP** (°C)**:** –143
MW: 91.97 **BP** (°C)**:** 2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.242E-04	8.500E-02	20	F300	1 0 0 0 1	

32. $CBrClF_2$
Bromochlorodifluoromethane
Halon 1211
Chlorodifluorobromomethane
Bromochlorodifluoromethine
RN: 353-59-3 **MP** (°C)**:**
MW: 165.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.555E-05	1.580E-02	0	G055	1 2 2 2 1	

33. CBr_3F
Tribromo-fluoro-methane
Methane, tribromofluoro-
Fluorotribromomethane
RN: 353-54-8 **MP** (°C)**:**
MW: 270.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-03	3.998E-01	25	O006	1 0 0 0 1	

34. CBr_4
Carbon tetrabromide
Tetrabromomethane
RN: 558-13-4 **MP** (°C)**:** 89
MW: 331.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.235E-04	2.399E-01	30	G029	1 0 2 2 1	
6.998E-04	2.321E-01	30	V009	1 0 0 0 0	

35. CClN
Cyanogen chloride
Chlorcyan
RN: 506-77-4 **MP** (°C)**:** –6
MW: 61.47 **BP** (°C)**:** 13.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.761E-01	6.000E+01	0	F300	1 0 0 0 0	

36. $CClN_3O_6$
Chlorotrinitromethane
Chlor-trinitro-methan
RN: 1943-16-4 **MP** (°C)**:**
MW: 185.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.186E-02	2.200E+00	20	F300	1 0 0 0 1	

37. CCl_2F_2
Dichlorodifluoromethane
Difluorodichloromethane
Freon 12
RN: 75-71-8 **MP** (°C)**:** –158
MW: 120.91 **BP** (°C)**:** –29.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-02	1.867E+00	21	M065	1 0 2 1 2	
2.316E-03	2.800E–01	25	M133	1 0 0 0 2	
2.316E-03	2.800E–01	25	P046	1 0 0 0 0	
2.315E-03	2.799E–01	25	R048	0 0 0 0 0	

38. CCl_3F
Trichlorofluoromethane
Fluorotrichloromethane
Freon 11
RN: 75-69-4 **MP** (°C)**:** –111
MW: 137.37 **BP** (°C)**:** 23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.401E+00	20	H041	0 0 0 0 0	
8.008E-03	1.100E+00	20	M133	1 0 0 0 2	
8.008E-03	1.100E+00	20	P046	1 0 0 0 0	
1.020E-02	1.401E+00	21	H041	0 0 0 0 0	

(*continued*)

38. CCl_3F (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.013E-03	1.101E+00	25	H041	0 0 0 0 0	
7.999E-03	1.099E+00	25	R048	0 0 0 0 0	
7.997E-03	1.099E+00	27	H041	0 0 0 0 0	
7.853E-03	1.079E+00	30	H041	0 0 0 0 0	
9.892E-03	1.359E+00	31	H041	0 0 0 0 0	
4.152E-03	5.703E–01	50	H041	0 0 0 0 0	
2.258E-03	3.102E–01	75	H041	0 0 0 0 0	

39. CCl_3NO_2
Chloropicrin
Chlorpikrin
RN: 76-06-2 **MP** (°C)**:** –64
MW: 164.38 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.270E+00	0	M161	1 0 0 0 2	
1.396E-02	2.295E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
1.186E-02	1.950E+00	20	G080	1 0 0 0 1	
9.718E-03	1.597E+00	20	M061	1 0 0 0 1	
1.214E-02	1.996E+00	20	P081	1 0 0 0 0	
9.874E-03	1.623E+00	25	F300	1 0 0 0 2	
1.217E-02	2.000E+00	ns	N013	0 0 0 0 2	

40. CCl_4
Carbon tetrachloride
Tetrachloromethane
Methane tetrachloride
RN: 56-23-5 **MP** (°C)**:** –23
MW: 153.82 **BP** (°C)**:** 76.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.306E-03	9.700E-01	0	H101	2 0 0 0 1	
5.002E-03	7.694E-01	15	G029	1 0 2 2 1	
5.002E-03	7.694E-01	15	J036	0 0 0 0 0	
5.197E-03	7.994E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
5.201E-03	8.000E-01	20	H101	2 0 0 0 1	
5.201E-03	8.000E-01	20	M040	1 0 0 1 2	
5.103E-03	7.850E-01	20	M133	1 0 0 0 2	
5.200E-03	7.999E-01	20	M312	1 0 0 0 2	
4.612E-03	7.095E-01	20	N038	1 0 0 1 2	
5.103E-03	7.850E-01	20	P046	1 0 0 0 0	

(*continued*)

40. CCl_4 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.494E-03	9.990E-01	25	B019	1 0 1 2 0	
4.920E-03	7.568E-01	25	B173	2 0 2 2 2	
5.000E-03	7.691E-01	25	G038	1 2 2 2 1	
5.000E-03	7.691E-01	25	G053	2 1 2 1 1	
5.197E-03	7.994E-01	25	G056	1 0 0 0 2	
5.197E-03	7.994E-01	25	L319	1 0 2 1 1	
5.201E-03	8.000E-01	25	M037	1 1 0 0 0	
5.197E-03	7.994E-01	25	M061	1 0 0 0 0	
1.820E-03	2.800E-01	25	M161	1 0 0 0 1	
5.006E-03	7.700E-01	25	M368	1 0 0 0 1	
1.038E-02	1.597E+00	25	N034	1 0 0 0 1	*sic*
5.556E-03	8.546E-01	25	S133	1 1 1 1 1	
5.262E-03	8.093E-01	30	G029	1 0 2 2 1	
5.526E-03	8.500E-01	30	H101	2 0 0 0 1	
5.296E-03	8.146E-01	30	V009	1 0 0 0 1	
5.201E-03	8.000E-01	ns	F071	0 1 2 1 2	
5.201E-03	8.000E-01	ns	H080	0 0 0 0 2	
3.249E-03	4.998E-01	ns	I306	0 0 0 0 0	
5.201E-03	8.000E-01	ns	M344	0 0 0 0 2	

41. CF_4

Carbon tetrafluoride
Tetrafluoromethane

RN: 75-73-0 **MP** (°C)**:** –184
MW: 88.00 **BP** (°C)**:** –128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.319E-04	2.041E-02	19.99	C115	2 0 2 2 2	
2.083E-04	1.833E-02	24.99	C115	2 0 2 2 2	
2.111E-04	1.858E-02	25	D055	1 0 0 0 1	
1.940E-04	1.707E-02	29.99	C115	2 0 2 2 2	

42. COS

Carbonyl sulfide
Kohlenoxidsulfid

RN: 463-58-1 **MP** (°C)**:** –138
MW: 60.07 **BP** (°C)**:** –50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.259E-02	3.760E+00	0	F300	1 0 0 0 2	
2.081E-02	1.250E+00	25	F300	1 0 0 0 2	

43. CO_2

Carbon dioxide
Carbonic acid gas
Carbonic anhydride

RN: 124-38-9 **MP** (°C)**:** –57
MW: 44.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.641E-02	3.803E+00	16	B109	1 0 0 0 2	unit assumed, *sic*
8.377E-02	3.687E+00	17	B109	1 0 0 0 2	unit assumed, *sic*
8.641E-02	3.803E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
8.123E-02	3.575E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
7.886E-02	3.471E+00	19	B109	1 0 0 0 2	unit assumed, *sic*
7.654E-02	3.369E+00	20	B109	1 0 0 0 2	unit assumed, *sic*
7.432E-02	3.271E+00	21	B109	1 0 0 0 2	unit assumed, *sic*
7.427E-02	3.269E+00	21	B109	1 0 0 0 2	unit assumed, *sic*
7.213E-02	3.174E+00	22	B109	1 0 0 0 2	unit assumed, *sic*
6.582E-02	2.897E+00	25	B109	1 0 0 0 2	unit assumed, *sic*
3.360E-02	1.479E+00	25	H124	1 0 0 1 2	
6.204E-02	2.730E+00	27	B109	1 0 0 0 2	unit assumed, *sic*
6.127E-02	2.696E+00	28	B109	1 0 0 0 2	unit assumed, *sic*
5.714E-02	2.515E+00	30	B109	1 0 0 0 2	unit assumed, *sic*

44. CS_2

Carbon disulfide
Carbon disulphide
Schwefelkohlenstoff

RN: 75-15-0 **MP** (°C)**:** –112
MW: 76.14 **BP** (°C)**:** 46.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-02	2.040E+00	0	F300	1 0 0 0 2	
3.257E-02	2.480E+00	0	H101	2 0 0 0 2	
2.883E-02	2.195E+00	20	C121	0 0 0 0 1	unit assumed, *sic*
2.351E-02	1.790E+00	20	F300	1 0 0 0 2	
2.850E-02	2.170E+00	20	G080	1 0 0 0 1	
2.844E-02	2.165E+00	20	M061	1 0 0 0 2	
3.850E-02	2.931E+00	20	N038	1 0 0 1 2	
2.889E-02	2.200E+00	22	P076	1 2 1 1 1	
3.746E-02	2.852E+00	25	L319	1 0 2 1 1	
2.036E-02	1.550E+00	30	F300	1 0 0 0 2	
2.889E-02	2.200E+00	32	M161	1 0 0 0 1	
2.627E-02	2.000E+00	ns	N013	0 0 0 0 2	

45. $C_2HBrClF_3$

Halothane
2-Bromo-2-chloro-1,1,1-trifluoroethane
Fluothane

RN: 151-67-7 **MP** (°C)**:** <25
MW: 197.39 **BP** (°C)**:** 50.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-02	3.438E+00	ns	R028	0 0 0 0 0	

46. C_2HCl_3

Trichloroethylene
Trichloroethene
Trichloro-ethylene
Ethinyl trichloride
Acetylene trichloride
1,1,2-Trichloroethylene

RN: 79-01-6 **MP** (°C)**:** –87
MW: 131.39 **BP** (°C)**:** 86.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-03	1.100E+00	20	M133	1 0 0 0 2	
9.654E-03	1.268E+00	20	P041	1 0 0 0 1	
8.372E-03	1.100E+00	20	P046	1 0 0 0 0	
7.603E-03	9.990E–01	25	A094	1 0 0 0 1	
1.120E-02	1.472E+00	25	B173	2 0 2 2 2	
8.363E-03	1.099E+00	25	G056	1 0 0 0 2	
8.372E-03	1.100E+00	25	M037	1 1 0 0 1	
1.040E-02	1.366E+00	25	M342	1 0 1 1 2	
8.372E-03	1.100E+00	25	M368	1 0 0 0 1	
8.363E-03	1.099E+00	25	N034	1 0 0 0 1	
3.032E-02	3.984E+00	25	N309	1 0 0 0 1	*sic*
5.656E-03	7.431E–01	30	M311	1 1 2 2 2	
9.274E-03	1.219E+00	37	P041	1 0 0 0 1	
8.363E-03	1.099E+00	ns	O006	0 0 0 0 1	

47. $C_2HCl_3O.H_2O$

Chloral (monhydrate)
Chloral-hydrat

RN: 302-17-0 **MP** (°C)**:** 57.0
MW: 165.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E+00	3.400E+02	0	F300	1 0 0 0 2	
4.837E+00	8.000E+02	11.30	F300	1 0 0 0 2	
5.629E+00	9.310E+02	38.10	F300	1 0 0 0 2	
4.794E+00	7.930E+02	rt	D021	0 0 1 1 2	

48. $C_2HCl_3O_2$
Trichloroacetic acid
TCA
RN: 76-03-9 **MP** (°C)**:** 57.5
MW: 163.39 **BP** (°C)**:** 196.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.338E+00	5.455E+02	25	B185	0 0 0 0 0	
5.685E+00	9.289E+02	25	B200	1 0 0 0 2	
2.146E+00	3.506E+02	25	F018	1 0 0 0 1	
4.024E+00	6.575E+02	25	K040	1 2 1 2 2	
1.000E+01	1.634E+03	ns	M163	0 0 0 0 0	EFG
2.146E+00	3.506E+02	ns	N013	0 0 0 0 1	

49. C_2HCl_5
Pentachloroethane
Pentachloro-ethane
Pentalin
Pentachlorethane
Ethane pentachloride
RN: 76-01-7 **MP** (°C)**:** –29
MW: 202.30 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-03	4.698E-01	20	V009	1 0 0 0 1	
2.470E-03	4.998E-01	25	G056	1 0 0 0 2	
2.472E-03	5.000E-01	25	M037	1 1 0 0 1	
2.373E-03	4.800E-01	ns	H123	0 0 0 0 0	
2.322E-03	4.698E-01	ns	O006	0 0 0 0 1	

50. C_2H_2
Acetylene
Acetylen
RN: 74-86-2 **MP** (°C)**:** –81
MW: 26.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.796E-02	2.030E+00	0	F300	1 0 0 0 2	*sic*
4.609E-02	1.200E+00	20	F300	1 0 0 0 2	*sic*
1.862E+01	4.848E+02	25	M101	1 0 0 0 2	
1.959E-02	5.100E-01	60	F300	1 0 0 0 1	*sic*

51. $C_2H_2Br_4$

sym-Tetrabromoethane
1,1,2,2-Tetrabrom-aethan
Acetylene tetrabromide
1,1,2,2-Tetrabromoethane
Tetrabromoacetylene

RN: 79-27-6 **MP** (°C)**:** 0
MW: 345.67 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-03	6.500E-01	30	F300	1 0 0 0 1	
1.879E-03	6.496E-01	30	O006	1 0 0 0 1	

52. $C_2H_2Cl_2$

Vinylidene chloride
1,1-Dichloroethylene

RN: 75-35-4 **MP** (°C)**:** –122.0
MW: 96.94 **BP** (°C)**:** 31.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.470E–02	2.394E+00	15	D086	1 0 2 2 1	
2.624E-02	2.544E+00	17	D086	1 0 2 2 2	
4.126E-03	4.000E-01	20	M133	1 0 0 0 2	
4.126E-03	4.000E-01	20	P046	1 0 0 0 0	
2.572E-02	2.494E+00	20.5	D086	1 0 2 2 1	
2.316E-02	2.245E+00	25	D086	1 0 2 2 2	
2.470E-02	2.394E+00	28.5	D086	1 0 2 2 1	
2.624E-02	2.544E+00	29.5	D086	1 0 2 2 2	
2.302E-02	2.232E+00	30	M311	1 1 2 2 2	
2.264E-02	2.195E+00	38.5	D086	1 0 2 2 1	
2.162E-02	2.096E+00	45	D086	1 0 2 2 1	
2.367E-02	2.295E+00	51	D086	1 0 2 2 1	
2.162E-02	2.096E+00	55	D086	1 0 2 2 1	
2.470E-02	2.394E+00	60	D086	1 0 2 2 1	
2.316E-02	2.245E+00	65	D086	1 0 2 2 2	
3.034E-02	2.941E+00	71	D086	1 0 2 2 2	
2.572E-02	2.494E+00	74.5	D086	1 0 2 2 1	
3.034E-02	2.941E+00	81	D086	1 0 2 2 2	
3.803E-02	3.686E+00	85.5	D086	1 0 2 2 1	
3.598E-02	3.488E+00	90.5	D086	1 0 2 2 1	

53. $C_2H_2Cl_2$
cis-Acetylene dichloride
cis-1,2-Dichloroethylene
cis-Dichlorethylene
RN: 156-59-2 **MP** (°C)**:** –80
MW: 96.94 **BP** (°C)**:** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E-02	3.500E+00	25	M037	1 1 0 0 1	

54. $C_2H_2Cl_2$
trans-Acetylene dichloride
trans-1,2-Dichloroethylene
trans-Dichlorethylene
RN: 156-60-5 **MP** (°C)**:** –50
MW: 96.94 **BP** (°C)**:** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.499E-02	6.300E+00	25	M037	1 1 0 0 1	

55. $C_2H_2Cl_3As$
Chlorovinyldichloroarsine
Chlorvinylarsin-dichlorid
RN: 541-25-3 **MP** (°C)**:**
MW: 207.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-03	5.000E-01	20	F300	1 0 0 0 0	

56. $C_2H_2Cl_4$
1,1,1,2-Tetrachloroethane
Ethane, 1,1,1,2-tetrachloro-
F 130α
TCA
HCC 130α
RN: 630-20-6 **MP** (°C)**:** –44
MW: 167.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.141E-03	1.199E+00	0	V009	1 0 0 0 2	
6.487E-03	1.089E+00	20	V009	1 0 0 0 2	
1.723E-02	2.892E+00	25	G056	1 0 0 0 2	
<1.66E-02	<2.79E+00	25.50	O005	2 0 2 2 1	
6.843E-03	1.149E+00	35	V009	1 0 0 0 2	
7.438E-03	1.248E+00	50	V009	1 0 0 0 2	

57. $C_2H_2Cl_4$
1,1,2,2-Tetrachloroethane
sym-Tetrachloroethane
RN: 79-34-5 **MP** (°C)**:** –36
MW: 167.85 **BP** (°C)**:** 146.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.924E-02	3.230E+00	20	C094	1 0 0 0 2	
1.758E-02	2.951E+00	23.5	S171	2 1 2 2 2	
1.770E-02	2.971E+00	25	B173	2 0 2 2 2	
1.782E-02	2.991E+00	25	F050	1 0 0 0 0	
1.728E-02	2.900E+00	25	M037	1 1 0 0 1	
1.737E-02	2.915E+00	30	M311	1 1 2 2 2	

58. $C_2H_2O_4$
Oxalic acid
Oxalsaeure
RN: 144-62-7 **MP** (°C)**:** 189
MW: 90.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.683E-01	3.316E+01	0	C066	1 0 1 1 2	
3.665E-01	3.300E+01	0	L041	1 0 0 1 1	
3.756E-01	3.382E+01	0	M043	1 0 0 0 1	
4.907E-01	4.418E+01	4.99	A339	0 0 0 0 0	
6.287E-01	5.660E+01	10	M043	1 0 0 0 1	
5.912E-01	5.323E+01	9.99	A339	0 0 0 0 0	
7.752E-01	6.979E+01	14.99	A339	0 0 0 0 0	
7.441E-01	6.700E+01	15	F066	2 2 2 2 1	
7.464E-01	6.720E+01	15	F300	1 0 0 0 2	
7.775E-01	7.000E+01	15	L041	1 0 0 1 1	
9.468E-01	8.524E+01	19.99	A339	0 0 0 0 0	
9.219E-01	8.300E+01	20	F066	2 2 2 2 1	
9.219E-01	8.300E+01	20	F300	1 0 0 0 1	
9.552E-01	8.600E+01	20	L041	1 0 0 1 1	
9.636E-01	8.676E+01	20	M043	1 0 0 0 1	
8.836E-01	7.956E+01	20	M171	1 0 0 0 1	
1.146E+00	1.032E+02	24.99	A339	0 0 0 0 0	
1.088E+00	9.800E+01	25	F066	2 2 2 2 1	
1.378E+00	1.240E+02	25	F317	2 1 1 1 2	
2.480E+00	2.233E+02	25	H084	1 0 0 0 2	
1.190E+00	1.071E+02	25	H430	0 0 0 0 0	
2.409E+00	2.169E+02	25	K040	1 0 2 1 2	
1.317E+00	1.186E+02	29.99	A339	0 0 0 0 0	
1.407E+00	1.266E+02	30	M043	1 0 0 0 2	
1.623E+00	1.461E+02	34.99	A339	0 0 0 0 0	
1.710E+00	1.540E+02	35	L041	1 0 0 1 2	
1.903E+00	1.713E+02	39.99	A339	0 0 0 0 0	

(*continued*)

58. $C_2H_2O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.973E+00	1.776E+02	40	M043	1 0 0 0 2	
2.199E+00	1.979E+02	44.99	A339	0 0 0 0 0	
2.527E+00	2.275E+02	49.99	A339	0 0 0 0 0	
2.150E+00	1.935E+02	50	C066	1 0 1 1 2	
2.821E+00	2.540E+02	50	L041	1 0 0 1 2	
2.867E+00	2.581E+02	54.99	A339	0 0 0 0 0	
3.121E+00	2.810E+02	59.99	A339	0 0 0 0 0	
3.410E+00	3.070E+02	60	M043	1 0 0 0 2	
3.661E+00	3.296E+02	64.99	A339	0 0 0 0 0	
4.121E+00	3.710E+02	65	L041	1 0 0 1 2	
3.583E+00	3.226E+02	80	C066	1 0 1 1 2	
5.084E+00	4.577E+02	80	M043	1 0 0 0 2	
6.059E+00	5.455E+02	90	F300	1 0 0 0 2	

59. $C_2H_2O_4.2H_2O$
Oxalic acid dihydrate
Ethanedioic acid, dihydrate
RN: 6153-56-6 **MP** (°C)**:** 101
MW: 126.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-02	1.820E+00	23	C038	2 2 2 2 0	EFG, 0.1N HCl
1.070E-02	1.349E+00	30	C038	2 2 2 2 0	EFG, 0.1N HCl
7.234E-03	9.120E-01	35	C038	2 2 2 2 0	EFG, 0.1N HCl

60. $C_2H_3Br_3O$
2,2,2-Tribromoethanol
2,2,2-Tribrom-aethanol
RN: 75-80-9 **MP** (°C)**:** 80
MW: 282.77 **BP** (°C)**:** 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-01	3.410E+01	40	F300	1 0 0 0 2	

61. C_2H_3Cl

Vinyl chloride
Chloroethylene

RN: 75-01-4 **MP** (°C)**:** –153.0
MW: 62.50 **BP** (°C)**:** –13.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	6.000E-02	10	M133	1 0 0 0 1	*sic*
9.600E-04	6.000E-02	10	P046	1 0 0 0 0	*sic*
1.506E-01	9.411E+00	15	D086	1 0 2 2 1	
1.576E-01	9.852E+00	16	D086	1 0 2 2 2	
1.081E-01	6.754E+00	20	N034	1 0 0 0 1	
1.451E-01	9.067E+00	20.5	D086	1 0 2 2 2	
<1.76E-02	<1.10E+00	25	I310	0 0 0 0 0	
1.396E-01	8.723E+00	26	D086	1 0 2 2 1	
1.411E-01	8.821E+00	29.5	D086	1 0 2 2 1	
1.490E-01	9.312E+00	35	D086	1 0 2 2 1	
1.411E-01	8.821E+00	41	D086	1 0 2 2 1	
1.396E-01	8.723E+00	46.5	D086	1 0 2 2 1	
6.717E-03	4.198E-01	50	M065	0 0 2 1 1	
1.506E-01	9.411E+00	55	D086	1 0 2 2 1	
1.459E-01	9.116E+00	65	D086	1 0 2 2 1	
1.553E-01	9.705E+00	72.5	D086	1 0 2 2 1	
1.584E-01	9.901E+00	80	D086	1 0 2 2 2	
1.772E-01	1.108E+01	85	D086	1 0 2 2 2	

62. $C_2H_3Cl_2NO_2$

1,1-Dichloro-1-nitroethane
Dichloronitroethane
Ethide

RN: 594-72-9 **MP** (°C)**:**
MW: 143.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.456E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
1.732E-02	2.494E+00	20	M061	1 0 0 0 1	

63. $C_2H_3Cl_3$
1,1,1-Trichloroethane
1,1,1-Trichloroethane
Trichloroethane
1,1,1-Trichloethane
RN: 71-55-6 **MP** (°C)**:** –35
MW: 133.41 **BP** (°C)**:** 74.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-02	1.587E+00	0	V009	1 0 0 0 2	
1.342E-02	1.790E+00	3.5	C094	1 0 0 0 2	
1.019E-02	1.360E+00	20	C094	1 0 1 0 2	
3.358E-02	4.480E+00	20	G056	1 0 0 0 2	
3.598E-03	4.800E-01	20	M133	1 0 0 0 2	
9.895E-03	1.320E+00	20	M368	1 0 0 0 1	
3.598E-03	4.800E-01	20	P046	1 0 0 0 0	
9.882E-03	1.318E+00	20	V009	1 0 0 0 2	
8.797E-03	1.174E+00	23.5	S171	2 1 2 2 2	
5.244E-03	6.995E-01	25	A094	1 0 0 0 0	
1.000E-02	1.334E+00	25	B173	2 0 2 2 2	
3.284E-02	4.381E+00	25	N309	1 0 0 0 1	*sic*
9.732E-03	1.298E+00	25	O006	1 0 0 0 1	
3.597E-03	4.798E-01	30	M311	1 1 2 2 2	
9.433E-03	1.258E+00	35	V009	1 0 0 0 2	
9.583E-03	1.278E+00	50	V009	1 0 0 0 2	
5.397E-03	7.200E-01	ns	H123	0 0 0 0 0	

64. $C_2H_3Cl_3$
1,1,2-Trichloroethane
1,1,2-β-Trichloroethane
RN: 79-00-5 **MP** (°C)**:** –37
MW: 133.41 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-02	4.638E+00	0	V009	1 0 0 0 2	
3.254E-02	4.341E+00	20	V009	1 0 0 0 2	
3.804E-02	5.074E+00	25	C119	2 2 2 2 2	
3.298E-02	4.400E+00	25	M037	1 1 0 0 1	
3.272E-02	4.365E+00	30	M311	1 1 2 2 2	
3.417E-02	4.559E+00	35	V009	1 0 0 0 2	
3.967E-02	5.292E+00	55	V009	1 0 0 0 2	

65. $C_2H_3FO_2$
Fluoroacetic acid
Essigsaeurefluorid
RN: 144-49-0 **MP** (°C)**:**
MW: 78.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.407E-04	5.000E-02	20	F300	1 0 0 0 0	

66. C_2H_3N
Acetonitrile
Acetonitril
RN: 75-05-8 **MP** (°C)**:** –45
MW: 41.05 **BP** (°C)**:** 81.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.95E+01	>8.00E+02	25	B019	1 0 1 2 0	

67. C_2H_3N
Methylisocyanide
Methyl-isocyanid
RN: 593-75-9 **MP** (°C)**:**
MW: 41.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E+00	9.100E+01	15	F300	1 0 0 0 1	

68. C_2H_3NS
Methyl isothiocyanate
Isothiocyanatomethane
RN: 556-61-6 **MP** (°C)**:** 35
MW: 73.12 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	7.600E+00	20	M161	1 0 0 0 1	
1.032E-01	7.543E+00	20	O300	1 0 0 0 1	
1.085E-01	7.937E+00	20	P081	1 0 0 0 0	

69. C_2H_4
Ethylene
Ethene
RN: 74-85-1 **MP** (°C)**:** –169
MW: 28.05 **BP** (°C)**:** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E+00	2.000E+02	0	R028	0 0 0 0 0	
3.240E+00	9.091E+01	25	R028	0 0 0 0 0	
3.187E+00	8.942E+01	30	C116	0 0 0 0 0	

70. C_2H_4BrCl
Ethylene chlorobromide
1-Bromo-2-chloroethane
RN: 107-04-0 **MP** (°C)**:** –17
MW: 143.42 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.778E-02	6.853E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

71. $C_2H_4Br_2$
1,2-Dibromoethane
Ethylene dibromide
Curafume
Haltox
1,2-Dibromaethan
RN: 106-93-4 **MP** (°C)**:** 9.97
MW: 187.87 **BP** (°C)**:** 131.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.777E-02	3.339E+00	0	V009	1 0 0 0 2	
2.078E-02	3.905E+00	15	G029	1 0 2 2 2	
1.874E-02	3.520E+00	20	C094	1 0 1 0 2	
2.279E-02	4.282E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
1.794E-02	3.370E+00	20	G080	1 0 0 0 1	
2.300E-02	4.321E+00	20	M312	1 0 0 0 1	
1.592E-02	2.991E+00	20	P081	1 0 0 0 0	
2.142E-02	4.024E+00	20	V009	1 0 0 0 2	
2.210E-02	4.153E+00	25	O006	1 0 0 0 2	
2.294E-02	4.310E+00	30	F300	1 0 0 0 2	
2.284E-02	4.292E+00	30	G029	1 0 2 2 2	
2.279E-02	4.282E+00	30	M061	1 0 0 0 1	
2.289E-02	4.300E+00	30	M161	1 0 0 0 1	
2.390E-02	4.490E+00	35	V009	1 0 0 0 2	
2.817E-02	5.292E+00	50	V009	1 0 0 0 2	

72. C_2H_4ClNO

Acetohydroxamic acid chloride
Acethydroximsaeure-chlorid
2-Chloroacetamide
Chloroacetamide
Chloressigsaeureamid
Essigsaeure-*N*-chloramid

RN: 79-07-2 **MP** (°C)**:** 119.5
MW: 93.51 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.624E-01	9.000E+01	24	F300	1 0 0 0 0	

73. $C_2H_4ClNO_2$

1-Chloro-1-nitroethane
1-Chloronitroethane

RN: 598-92-5 **MP** (°C)**:**
MW: 109.51 **BP** (°C)**:** 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.638E-02	3.984E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
3.638E-02	3.984E+00	20	M061	1 0 0 0 0	

74. $C_2H_4Cl_2$

Ethylidene chloride
1,1-Dichloraethan
1,1-Dichloroethane

RN: 75-34-3 **MP** (°C)**:** –97
MW: 98.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-02	6.600E+00	0	F300	1 0 0 0 1	
6.629E-02	6.560E+00	0	H101	2 0 0 0 2	
5.967E-02	5.905E+00	0	V009	1 0 0 0 2	
5.558E-02	5.500E+00	20	F300	1 0 0 0 1	
5.558E-02	5.500E+00	20	H101	2 0 0 0 2	
5.087E-02	5.035E+00	20	V009	1 0 0 0 2	
5.110E-02	5.057E+00	25	G038	1 2 2 2 2	
5.110E-02	5.057E+00	25	G053	2 2 2 1 2	
5.457E-02	5.400E+00	30	F300	1 0 0 0 1	
4.885E-02	4.834E+00	30	M300	1 1 2 2 2	
4.637E-02	4.589E+00	30	M311	1 1 2 2 2	
5.397E-02	5.341E+00	30	N034	1 0 0 0 2	
4.847E-02	4.797E+00	35	V009	1 0 0 0 2	
5.217E-02	5.163E+00	50	V009	1 0 0 0 2	

75. $C_2H_4Cl_2$

Ethylene dichloride
1,2-Dichloraethan

RN: 107-06-2 **MP** (°C)**:** –35
MW: 98.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.095E-02	9.000E+00	0	F300	1 0 0 0 0	
9.317E-02	9.220E+00	0	H101	2 0 0 0 2	
9.232E-02	9.136E+00	0	L103	1 0 0 0 2	unit assumed
8.745E-02	8.654E+00	0	V009	1 0 0 0 2	
8.735E-02	8.645E+00	15	G029	1 0 2 2 2	
8.539E-02	8.450E+00	20	C094	1 0 1 0 2	
8.716E-02	8.625E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
8.716E-02	8.625E+00	20	D052	1 1 0 0 1	
8.716E-02	8.625E+00	20	G056	1 0 0 0 2	
8.781E-02	8.690E+00	20	H101	2 0 0 0 2	
8.706E-02	8.615E+00	20	L103	1 0 0 0 2	unit assumed
8.706E-02	8.615E+00	20	M061	1 0 0 0 2	
8.616E-02	8.527E+00	20	M062	1 0 0 0 1	
8.892E-02	8.800E+00	20	M133	1 0 0 0 2	
8.716E-02	8.625E+00	20	O006	1 0 0 0 1	
8.892E-02	8.800E+00	20	P046	1 0 0 0 0	
8.507E-02	8.419E+00	20	V009	1 0 0 0 2	
8.070E-02	7.986E+00	25	B173	2 0 2 2 2	
1.060E-01	1.049E+01	25	C119	2 2 2 2 2	
8.690E-02	8.600E+00	25	F300	1 0 0 0 2	
8.740E-02	8.649E+00	25	G038	1 2 2 2 2	
8.740E-02	8.649E+00	25	G053	2 1 2 1 2	
8.488E-02	8.400E+00	25	M037	1 1 0 0 1	
9.013E-02	8.920E+00	30	G029	1 0 2 2 1	
8.954E-02	8.861E+00	30	L103	1 0 0 0 2	unit assumed
3.543E-02	3.506E+00	30	M311	1 1 2 2 2	
8.964E-02	8.871E+00	35	V009	1 0 0 0 2	
1.030E-01	1.019E+01	56	V009	1 0 0 0 2	
8.716E-02	8.625E+00	72	B197	0 0 0 0 0	at bp of 72 °C
5.927E-02	5.865E+00	89.3	B197	0 0 0 0 0	at bp of 89.3 °C
4.327E-02	4.282E+00	92.3	B197	0 0 0 0 0	at bp of 92.3 °C
3.324E-02	3.289E+00	94	B197	0 0 0 0 0	at bp of 94 °C
1.312E-02	1.298E+00	98	B197	0 0 0 0 0	at bp of 98 °C
4.345E-02	4.300E+00	rt	M161	0 0 0 0 1	

76. $C_2H_4F_2$

1,1-Difluoroethane
Ethylidene fluoride

RN: 75-37-6 **MP** (°C)**:** –117
MW: 66.05 **BP** (°C)**:** –24.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.132E-02	5.371E+00	0	M065	0 0 2 1 2	

77. $C_2H_4N_2O_2$
Oxamide
Oxalsaeure-diamid
RN: 471-46-5 **MP** (°C)**:**
MW: 88.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-03	3.700E-01	7.30	F300	1 0 0 0 1	
7.040E-02	6.200E+00	100	F300	1 0 0 0 1	

78. $C_2H_4N_4$
Amitrole
3-Amino-1,2,4-triazole
3-Amino-*s*-triazole
ATA
Aminotriazole
RN: 61-82-5 **MP** (°C)**:** 159.0
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	2.188E+02	23	M061	1 0 0 0 1	
2.602E+00	2.188E+02	25	B185	0 0 0 0 0	
2.602E+00	2.188E+02	25	B200	1 0 0 0 1	
2.602E+00	2.188E+02	25	I310	0 0 0 0 0	
3.330E+00	2.800E+02	25	M161	1 0 0 0 2	
2.602E+00	2.188E+02	ns	B100	0 0 0 0 1	
3.162E+00	2.659E+02	ns	M163	0 0 0 0 0	EFG

79. $C_2H_4N_4$
Dicyanodiamide
Dicyandiamid
Dicyandiamide
RN: 461-58-5 **MP** (°C)**:** 210
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E-01	1.283E+01	0	M043	1 0 0 0 1	
2.218E-01	1.865E+01	10	M043	1 0 0 0 1	
2.617E-01	2.200E+01	13	F300	1 0 0 0 1	
3.688E-01	3.101E+01	20	M043	1 0 0 0 1	
4.876E-01	4.100E+01	25	F300	1 0 0 0 1	
4.717E-01	3.966E+01	25.0	H037	1 2 2 1 2	
5.663E-01	4.762E+01	30	M043	1 0 0 0 1	
8.565E-01	7.201E+01	39.9	H037	1 2 2 1 2	
8.606E-01	7.236E+01	40	M043	1 0 0 0 1	
1.255E+00	1.055E+02	49.8	H037	1 2 2 1 2	

(*continued*)

79. $C_2H_4N_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.899E+00	1.597E+02	60	M043	1 0 0 0 1	
1.878E+00	1.579E+02	60.1	H037	1 2 2 1 2	
2.236E+00	1.880E+02	60.10	F300	1 0 0 0 2	
2.978E+00	2.504E+02	74.5	H037	1 2 2 1 2	
3.275E+00	2.754E+02	80	M043	1 0 0 0 1	
1.492E-01	1.254E+01	.0	H037	1 2 2 1 2	

80. $C_2H_4N_4O_2S_2$
2-Amino-1,3,4-thiadiazole-5-sulfonamide
5-Amino-1,3,4-thiadiazol-2-sulfonamide
5-Amino-1,3,4-thiadiazole-2-sulfonamide
CL 5343
Tio-urasin
RN: 14949-00-9 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-02	4.739E+00	15	K024	1 2 1 1 2	

81. $C_2H_4O_2$
Acetic acid glacial
Acetic acid
Essigsaeure
RN: 64-19-7 **MP** (°C)**:** 16.7
MW: 60.05 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E+01	6.029E+02	25	H084	1 0 0 0 2	

82. $C_2H_4O_2$
Methyl formate
Methyl methanoate
Formic acid methyl ester
RN: 107-31-3 **MP** (°C)**:** –99.8
MW: 60.05 **BP** (°C)**:** 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.80E+00	+2.28E+02	ns	S460	0 0 0 0 0	

83. $C_2H_4O_3$
Glycolic acid
Glykolsaeure
RN: 79-14-1 **MP** (°C)**:** 80
MW: 76.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.084E+00	4.627E+02	6.99	A340	0 0 0 0 0	
6.913E+00	5.258E+02	10.89	A340	0 0 0 0 0	
7.894E+00	6.004E+02	20.69	A340	0 0 0 0 0	
8.015E+00	6.096E+02	24.99	A340	0 0 0 0 0	
8.168E+00	6.212E+02	30.09	A340	0 0 0 0 0	
8.296E+00	6.309E+02	35.99	A340	0 0 0 0 0	
8.400E+00	6.388E+02	39.99	A340	0 0 0 0 0	
8.533E+00	6.489E+02	47.99	A340	0 0 0 0 0	
8.536E+00	6.492E+02	48.99	A340	0 0 0 0 0	
8.654E+00	6.582E+02	54.99	A340	0 0 0 0 0	
8.721E+00	6.632E+02	59.49	A340	0 0 0 0 0	
8.808E+00	6.698E+02	64.49	A340	0 0 0 0 0	
8.866E+00	6.743E+02	69.99	A340	0 0 0 0 0	
8.932E+00	6.793E+02	74.99	A340	0 0 0 0 0	
8.968E+00	6.820E+02	79.89	A340	0 0 0 0 0	
9.016E+00	6.857E+02	84.49	A340	0 0 0 0 0	
9.043E+00	6.877E+02	88.09	A340	0 0 0 0 0	

84. C_2H_5Br
Bromoethane
Ethyl bromide
Aethylbromid
RN: 74-96-4 **MP** (°C)**:** –119
MW: 108.97 **BP** (°C)**:** 38.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.792E-02	1.067E+01	0	H101	2 0 0 0 2	
8.810E-02	9.600E+00	17.5	F001	1 0 1 2 2	
8.810E-02	9.600E+00	17.5	S006	1 0 0 0 2	
8.259E-02	9.000E+00	20	F300	1 0 0 0 0	
8.388E-02	9.140E+00	20	H101	2 0 0 0 2	
8.185E-02	8.920E+00	20	H127	1 0 0 0 0	
8.127E-02	8.856E+00	30	V009	1 0 0 0 1	

85. C_2H_5Cl
Ethyl chloride
Aethylchlorid
Chloroethane
Monochloroethane
RN: 75-00-3 **MP** (°C)**:** –139.0
MW: 64.52 **BP** (°C)**:** 12.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-02	4.500E+00	0	M037	1 1 0 0 1	
6.898E-02	4.450E+00	0	V009	1 0 0 0 2	
7.865E-02	5.074E+00	20	G056	1 0 0 0 2	
8.846E-02	5.707E+00	20	N034	1 0 0 0 2	
8.900E-02	5.742E+00	ns	F001	0 0 1 2 2	
8.433E-02	5.440E+00	ns	R028	0 0 0 0 0	

86. C_2H_5I
Iodoethane
Ethyl iodide
Aethyliodid
Iodaethan
RN: 75-03-6 **MP** (°C)**:** –108
MW: 155.97 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-02	4.410E+00	0	H101	2 0 0 0 2	
2.571E-02	4.010E+00	20	F300	1 0 0 0 2	
2.584E-02	4.030E+00	20	H101	2 0 0 0 2	
2.510E-02	3.915E+00	20	M171	1 0 0 0 2	
2.510E-02	3.915E+00	22.5	F001	1 0 1 2 2	
2.510E-02	3.915E+00	22.5	S006	1 0 0 0 2	
2.580E-02	4.024E+00	30	G029	1 0 2 2 2	
2.661E-02	4.150E+00	30	H101	2 0 0 0 2	
2.580E-02	4.023E+00	30	V009	1 0 0 0 2	

87. C_2H_5N
Ethylenimine
Aethylenimin
Aziridine
Ethyleneimine
Dimethyleneimine
RN: 151-56-4 **MP** (°C)**:** –78
MW: 43.07 **BP** (°C)**:** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.117E-01	9.116E+00	20	P315	0 0 0 0 0	

88. C_2H_5NO
Acetamide
Acetamid
RN: 60-35-5 **MP** (°C)**:** 81.0
MW: 59.07 **BP** (°C)**:** 222.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E+01	6.030E+02	.3	F300	1 0 0 0 2	
8.342E+00	4.927E+02	0	M022	1 0 0 0 2	
9.816E+00	5.798E+02	0	M043	1 0 0 0 2	
1.077E+01	6.364E+02	10	M043	1 0 0 0 2	
1.165E+01	6.880E+02	20	F300	1 0 0 0 2	
9.691E+00	5.724E+02	20	M022	1 0 0 0 2	
1.180E+01	6.970E+02	20	M043	1 0 0 0 2	
1.194E+01	7.050E+02	24.50	F300	1 0 0 0 2	
3.386E+01	2.000E+03	25	I310	0 0 0 0 0	
1.280E+01	7.561E+02	30	M043	1 0 0 0 2	
1.093E+01	6.455E+02	40	M022	1 0 0 0 2	
1.379E+01	8.148E+02	40	M043	1 0 0 0 2	
1.208E+01	7.138E+02	60	M022	1 0 0 0 2	
1.515E+01	8.947E+02	60	M043	1 0 0 0 2	
8.358E+00	4.937E+02	rt	D021	0 0 1 1 2	

89. $C_2H_5NO_2$
Glycine
Glycin
Glycocoll
RN: 56-40-6 **MP** (°C)**:** 245
MW: 75.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E+00	1.252E+02	0	D018	2 2 2 1 2	
1.656E+00	1.243E+02	0	M043	1 0 0 0 2	
1.905E+00	1.430E+02	10	C347	0 0 0 0 0	EFG
2.032E+00	1.525E+02	10	M043	1 0 0 0 2	
3.025E+00	2.271E+02	15	D349	2 1 1 2 2	
1.710E+00	1.284E+02	15	G081	1 0 1 1 2	
3.009E+00	2.259E+02	20	B032	1 2 2 2 2	
2.336E+00	1.754E+02	20	C347	0 0 0 0 0	EFG
3.180E+00	2.387E+02	20	D349	2 1 1 2 2	
2.447E+00	1.837E+02	20	M043	1 0 0 0 2	
2.616E+00	1.964E+02	21	P045	1 0 2 1 2	
2.127E+00	1.597E+02	22.9	Y412	0 0 0 0 0	
2.741E+00	2.058E+02	24.99	C404	2 1 2 2 1	
3.316E+00	2.489E+02	25	B032	1 2 2 2 2	
2.885E+00	2.166E+02	25	C018	0 0 0 0 0	
2.700E-03	2.027E-01	25	C405	2 1 2 2 2	intrinsic zwit

(*continued*)

89. $C_2H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.329E+00	2.499E+02	25	D016	1 0 0 0 2	
2.691E+00	2.020E+02	25	D018	2 2 2 1 2	
2.663E+00	1.999E+02	25	D041	1 0 0 0 2	
3.325E+00	2.496E+02	25	D349	2 1 1 2 2	
2.886E+00	2.166E+02	25	E015	1 2 1 1 2	
2.660E+00	1.997E+02	25	F300	1 0 0 0 2	
2.664E+00	2.000E+02	25	G092	2 1 1 1 1	
2.664E+00	2.000E+02	25	G315	0 0 0 0 0	
2.526E+00	1.897E+02	25	K031	2 1 2 1 2	
2.886E+00	2.166E+02	25	M024	1 2 0 1 2	
3.334E+00	2.503E+02	25	M029	2 2 2 2 2	
2.760E+00	2.072E+02	25	N001	0 0 0 0 0	EFG
2.900E+00	2.177E+02	25	N012	2 0 2 1 2	
2.544E+00	1.910E+02	25	O316	1 0 1 2 2	
2.664E+00	2.000E+02	25	O316	1 0 1 2 2	
2.715E+00	2.038E+02	25	O317	1 0 1 2 2	
3.330E+00	2.500E+02	25.1	N024	0 0 0 0 0	
3.352E+00	2.516E+02	25.1	N025	0 0 0 0 0	
3.342E+00	2.509E+02	25.1	N026	0 0 0 0 0	
2.673E+00	2.006E+02	25.1	N027	1 1 2 2 2	
2.220E+00	1.667E+02	25.3	Y412	0 0 0 0 0	
3.144E+00	2.360E+02	27	D036	0 0 0 0 0	
3.074E+00	2.308E+02	27	D036	0 0 0 0 0	
2.312E+00	1.736E+02	29.2	Y412	0 0 0 0 0	
3.630E+00	2.725E+02	29.80	B032	1 2 2 1 2	
2.737E+00	2.054E+02	30	C347	0 0 0 0 0	EFG
2.832E+00	2.126E+02	30	M043	1 0 0 0 1	
3.106E+00	2.332E+02	34.99	C404	2 1 2 2 1	
2.491E+00	1.870E+02	36.8	Y412	0 0 0 0 0	
2.578E+00	1.935E+02	38.2	Y412	0 0 0 0 0	
3.109E+00	2.334E+02	40	C347	0 0 0 0 0	EFG
3.305E+00	2.481E+02	40	M043	1 0 0 0 1	
3.538E+00	2.656E+02	44.99	C404	2 1 2 2 1	
2.749E+00	2.063E+02	45.5	Y412	0 0 0 0 0	
3.547E+00	2.662E+02	50	C347	0 0 0 0 0	EFG
3.816E+00	2.865E+02	50	D018	2 2 2 1 2	
3.745E+00	2.811E+02	50	F300	1 0 0 0 2	
3.921E+00	2.943E+02	60	C347	0 0 0 0 0	EFG
4.134E+00	3.103E+02	60	M043	1 0 0 0 1	
4.215E+00	3.164E+02	70	C347	0 0 0 0 0	EFG
4.863E+00	3.650E+02	75	D018	2 2 2 1 2	
4.693E+00	3.523E+02	75	D041	1 0 0 0 2	
4.693E+00	3.523E+02	75	F300	1 0 0 0 2	
4.517E+00	3.390E+02	80	C347	0 0 0 0 0	EFG
4.836E+00	3.631E+02	80	M043	1 0 0 0 1	
4.753E+00	3.568E+02	90	C347	0 0 0 0 0	EFG
4.911E+00	3.686E+02	100	C347	0 0 0 0 0	EFG
5.353E+00	4.018E+02	100	F300	1 0 0 0 2	

(*continued*)

89. $C_2H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.485E+00	4.118E+02	100	M043	1 0 0 0 1	
5.353E+00	4.018E+02	99.99	P349	0 0 0 0 0	
1.612E+00	1.210E+02	—	C347	0 0 0 0 0	EFG
6.661E+00	5.000E+02	ns	D072	0 0 0 0 0	
4.499E+00	3.377E+02	rt	D021	0 0 1 1 2	

90. $C_2H_5NO_2$
Nitroethane
Nitroetan
RN: 79-24-3 **MP** (°C)**:** –50
MW: 75.07 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.736E-01	4.306E+01	20	C121	1 0 0 0 1	unit assumed, *sic*
6.404E-01	4.807E+01	25	M346	2 1 1 1 2	

91. $C_2H_5NO_2$
Methyl carbamate
Carbamidsaeure-methyl ester
Methyl urethane
RN: 598-55-0 **MP** (°C)**:** 52
MW: 75.07 **BP** (°C)**:** 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.125E+00	6.850E+02	11	F300	1 0 0 0 2	
9.119E+00	6.845E+02	11	I314	0 0 0 0 0	
9.200E+00	6.906E+02	15.50	F001	1 0 1 0 2	
5.462E+00	4.100E+02	15.50	F300	1 0 0 0 1	

92. $C_2H_5NO_2$
Glycolamide
2-Hydroxyacetamide
2-Hydroxyacetimidic acid
Glycolic amide
Glycolic acid amide
RN: 598-42-5 **MP** (°C)**:**
MW: 75.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.509E+00	4.135E+02	25	M008	1 0 0 0 2	

93. C_2H_5NS
Thiacetamide
Thioessigsaeureamid
Thioacetamide
Acetothioamide
Ethanethioamide
RN: 62-55-5 **MP** (°C)**:** 113
MW: 75.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.865E+00	1.402E+02	25	I310	0 0 0 0 0	

94. $C_2H_5N.2H_2O$
Ethyleneimine (dihydrate)
Aziridine (dihydrate)
RN: 151-56-4 **MP** (°C)**:**
MW: 79.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-02	5.411E+00	20	P315	0 0 0 0 0	

95. $C_2H_5N_3O_2$
Methylnitrosourea
MNU
Nitrosomethylurea
RN: 684-93-5 **MP** (°C)**:** 123
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.443E+01	24	M031	1 1 1 1 1	
1.413E-01	1.456E+01	ns	R424	0 0 0 0 0	

96. $C_2H_5N_3O_2$
Biuret
Carbamylurea
RN: 108-19-0 **MP** (°C)**:**
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-01	1.200E+01	0	F300	1 0 0 0 2	
1.475E-01	1.520E+01	15	F300	1 0 0 0 2	
3.104E+00	3.200E+02	106	F300	1 0 0 0 1	

97. $C_2H_5N_5O_3$
N-Methyl-*N′*-nitro-*N*-nitrosoguanidine
MNNG
1-Methyl-3-nitro-1-nitrosoguanidine
RN: 70-25-7 **MP** (°C)**:** 118
MW: 147.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.38E-02	<4.98E+00	ns	I307	0 0 0 0 0	

98. $C_2H_5O_5P$
Phosphoacetic acid
Phosphor carboxymethyl-phosphonsaeure
Phosphonoacetic acid
RN: 4408-78-0 **MP** (°C)**:** 144.5
MW: 140.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E+00	3.920E+02	0	F300	1 0 0 0 2	
2.800E+00	3.921E+02	0	N028	1 0 0 0 2	

99. $C_2H_5O_5As$
Arsonoacetic acid
Arsono-essigsaeure
RN: 107-38-0 **MP** (°C)**:** 152
MW: 183.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E+00	4.000E+02	18	F300	1 0 0 0 1	

100. C_2H_6
Ethane
Aethan
RN: 74-84-0 **MP** (°C)**:** –172
MW: 30.07 **BP** (°C)**:** –88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-01	7.779E+00	0	C075	1 0 1 0 1	
4.157E-03	1.250E-01	0	F300	1 0 0 0 2	
3.601E-03	1.083E-01	4.99	C115	2 0 2 2 2	
2.903E-03	8.730E-02	9.99	C115	2 0 2 2 2	
2.465E-03	7.413E-02	14.99	C115	2 0 2 2 2	

(*continued*)

100. C_2H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-03	6.682E-02	19.8	G058	1 0 0 0 2	
2.129E-03	6.401E-02	19.99	C115	2 0 2 2 2	
1.929E-03	5.800E-02	20	F300	1 0 0 0 1	
1.850E-03	5.563E-02	24.99	C115	2 0 2 2 2	
2.009E-03	6.040E-02	25	M001	2 1 2 2 2	
2.009E-03	6.040E-02	25	M002	2 2 1 2 2	
1.760E-03	5.292E-02	25	M102	1 2 2 1 2	
1.620E-03	4.871E-02	29.99	C115	2 0 2 2 2	
7.981E-04	2.400E-02	60	F300	1 0 0 0 1	

101. C_2H_6O

Methyl ether
Dimethyl ether
Dimethylaether

RN: 115-10-6 **MP** (°C)**:** –138
MW: 46.07 **BP** (°C)**:** –23.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.476E+00	6.800E+01	18	F300	1 0 0 0 1	
5.669E+00	2.612E+02	24	M065	1 0 2 1 2	

102. $C_2H_6O_2$

Ethylene glycol
Glycol
1,2-Ethandiol

RN: 107-21-1 **MP** (°C)**:** –13
MW: 62.07 **BP** (°C)**:** 197.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.710E+00	4.165E+02	4.50	C022	1 2 0 0 2	
5.562E-01	3.452E+01	25	B004	0 0 0 0 0	

103. $C_2H_6O_3S$

Methyl methanesulphonate
Methyl mesylate
Methanesulfonic acid methyl ester

RN: 66-27-3 **MP** (°C)**:** 20
MW: 110.13 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.513E+00	1.667E+02	25	I310	0 0 0 0 0	

104. $C_2H_6O_4S$

Dimethyl sulfate
Sulfuric acid dimethyl ester

RN: 77-78-1 **MP** (°C)**:** –27
MW: 126.13 **BP** (°C)**:** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-01	2.800E+01	18	B078	1 0 0 0 1	
2.159E-01	2.724E+01	18	D049	1 2 0 0 1	

105. C_2H_7N

Ethylamine
Aethylamin

RN: 75-04-7 **MP** (°C)**:** –81
MW: 45.08 **BP** (°C)**:** 16.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.686E-02	1.211E+00	25	B004	0 0 0 0 0	

106. $C_2H_7NO_3S$

Taurine
Taurin

RN: 107-35-7 **MP** (°C)**:** 328
MW: 125.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-01	3.754E+01	0	M043	1 0 0 0 1	
4.523E-01	5.660E+01	10	M043	1 0 0 0 1	
4.842E-01	6.060E+01	12	F300	1 0 0 0 2	
3.919E-01	4.905E+01	15	G081	1 0 1 1 2	
6.448E-01	8.070E+01	20	F300	1 0 0 0 2	
6.463E-01	8.088E+01	20	M043	1 0 0 0 1	
4.700E-01	5.882E+01	24	D031	1 0 0 0 2	
7.580E-01	9.486E+01	25	D041	1 0 0 0 2	
8.815E-01	1.103E+02	30	M043	1 0 0 0 2	
1.149E+00	1.438E+02	40	M043	1 0 0 0 2	
1.719E+00	2.151E+02	60	M043	1 0 0 0 2	
1.985E+00	2.484E+02	70	F300	1 0 0 0 2	
2.105E+00	2.634E+02	75	D041	1 0 0 0 2	
2.217E+00	2.775E+02	80	M043	1 0 0 0 2	
2.506E+00	3.137E+02	100	M043	1 0 0 0 2	

107. $C_2H_7O_2As$
Cacodylic acid
Dimethylarsinsaeure
Kakodylsaeure
Arsine oxide, hydroxydimethyl-
Cacodylic acid
RN: 75-60-5 **MP** (°C)**:** 195
MW: 138.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.899E+00	4.001E+02	20	B200	1 0 0 0 2	
3.287E+00	4.536E+02	22	B185	0 0 0 0 0	
3.290E+00	4.540E+02	22	F300	1 0 0 0 2	
4.961E+00	6.845E+02	25	D305	1 0 0 0 2	
1.449E+01	2.000E+03	25	M161	1 0 0 0 0	

108. C_2H_7As
Ethylarsine
Aethylarsin
Arsen
RN: 593-59-9 **MP** (°C)**:**
MW: 106.00 **BP** (°C)**:** 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	1.300E-01	19	F300	1 0 0 0 1	

109. $C_2Cl_2F_4$
1,2-Dichlorotetrafluoroethane
CFC-114
sym-Dichlorotetrafluoroethane
Halon 242
1,2-Dichloro-1,1,2,2-tetrafluoroethane
Cryofluorane
RN: 76-14-2 **MP** (°C)**:** –94
MW: 170.92 **BP** (°C)**:** 3.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-04	1.300E-01	25	R048	0 0 0 0 0	

110. $C_2Cl_3F_3$
1,1,2-Trichloro-1,2,2-trifluoroethane
Freon 113
Fluorocarbon 113
Halocarbon 113
RN: 76-13-1 **MP** (°C)**:** –36.4
MW: 187.38 **BP** (°C)**:** 47.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.071E-04	1.700E-01	25	R048	0 0 0 0 0	

111. C_2Cl_4
Tetrachloroethylene
Ethylene tetrachloride
Perchloroethylene
Tetrachloroethene
Tetrachloro-ethylene
PERC
RN: 127-18-4 **MP** (°C)**:** –22
MW: 165.83 **BP** (°C)**:** 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-03	2.000E-01	20	C094	1 0 1 0 2	
1.206E-03	2.000E-01	20	C121	0 0 0 0 0	unit assumed, *sic*
9.045E-04	1.500E-01	20	M133	1 0 0 0 2	
9.045E-04	1.500E-01	20	P046	1 0 0 0 0	
9.044E-04	1.500E-01	25	A094	1 0 0 0 1	
2.920E-03	4.842E-01	25	B173	2 0 2 2 2	
1.206E-03	2.000E-01	25	C119	2 2 2 2 2	
2.412E-03	4.000E-01	25	F071	1 1 2 1 2	
9.044E-04	1.500E-01	25	G056	1 0 0 0 2	
9.045E-04	1.500E-01	25	M037	1 1 0 0 1	
9.045E-04	1.500E-01	25	M368	1 0 0 0 1	
9.044E-04	1.500E-01	25	N034	1 0 0 0 1	
2.412E-03	4.000E-01	ns	M344	0 0 0 0 2	
9.044E-04	1.500E-01	ns	O006	0 0 0 0 1	

112. C_2Cl_6
Hexachloroethane
1,1,1,2,2,2-Hexachloroethane
Avlothane
Distopin
Distopan
Distokal
RN: 67-72-1 **MP** (°C)**:** 187
MW: 236.74 **BP** (°C)**:** 186.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-05	7.700E-03	20	M339	2 2 2 2 1	
2.112E-04	5.000E-02	22.3	M037	1 1 0 0 0	
1.148E-04	2.718E-02	ns	R427	0 0 0 0 0	

113. C_2N_2
Cyanogen
Dicyan
RN: 460-19-5 **MP** (°C)**:**
MW: 52.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E+01	8.182E+02	20	F300	1 0 0 0 1	

114. $C_2N_4S_2$
Cyanogen azidodithiocarbonate
RN: **MP** (°C)**:**
MW: 144.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-02	1.500E+00	0	A055	0 0 0 0 2	

115. $C_2N_6S_4$
Thioperoxydicarbonic diazide
Azidoschwefel-kohlenstoff
Azidocarbonicdisulfide
RN: 148832-09-1 **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E-03	3.000E-01	25	F300	1 0 0 0 0	

116. $C_3H_2Cl_2N_2O_2$
1,3-Dichlorohydantoin
2,4-Imidazolidinedione, 1,3-dichloro-
RN: 2958-99-8 **MP** (°C)**:**
MW: 168.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.114E-02	6.951E+00	20	B080	1 0 1 1 0	
8.171E-02	1.381E+01	40	B080	1 0 1 1 1	

117. $C_3H_2N_2$
Malononitrile
Malonsaeure-dinitril
RN: 109-77-3 **MP** (°C)**:** 32
MW: 66.06 **BP** (°C)**:** 218.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E+00	1.176E+02	20	F300	1 0 0 0 2	
1.778E+00	1.175E+02	ns	R424	0 0 0 0 0	

118. $C_3H_2N_2O_3$
Parabanic acid
Parabansaeure
RN: 120-89-8 **MP** (°C)**:**
MW: 114.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.945E-01	4.500E+01	8	F300	1 0 0 0 1	

119. $C_3H_3Cl_3O_3$
β,β,β-Trichlorolactic acid
β,β,β-Trichlor-milchsaeure
RN: 599-01-9 **MP** (°C)**:**
MW: 193.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E+00	4.380E+02	25	F300	1 0 0 0 2	

120. C_3H_3N

Acrylonitrile
Propenitrile

RN: 107-13-1 **MP** (°C)**:** –83.5
MW: 53.06 **BP** (°C)**:** 77.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E+00	6.716E+01	0	D046	0 0 0 0 0	
1.266E+00	6.716E+01	0	D046	2 2 0 0 1	EFG
1.282E+00	6.803E+01	20	D046	0 0 0 0 0	
1.282E+00	6.803E+01	20	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	0 0 0 0 0	
1.298E+00	6.890E+01	25	L096	1 2 0 2 1	
1.413E+00	7.500E+01	25	M161	1 0 0 0 1	
1.315E+00	6.977E+01	28	D046	2 2 0 0 1	EFG
1.347E+00	7.149E+01	36	D046	2 2 0 0 1	EFG
1.364E+00	7.236E+01	39	D046	2 2 0 0 1	EFG
1.388E+00	7.365E+01	41	D046	2 2 0 0 2	EFG
1.508E+00	8.004E+01	49	D046	2 2 0 0 1	EFG
1.508E+00	8.004E+01	53	D046	2 2 0 0 1	EFG
1.540E+00	8.173E+01	59	D046	2 2 0 0 1	EFG
1.603E+00	8.509E+01	63	D046	2 2 0 0 1	EFG
1.760E+00	9.338E+01	65	A324	2 2 2 1 2	
1.651E+00	8.759E+01	68	D046	2 2 0 0 0	EFG
1.721E+00	9.132E+01	72	D046	2 2 0 0 0	EFG
1.869E+00	9.918E+01	80	D046	2 2 0 0 0	EFG
1.974E+00	1.047E+02	85	D046	2 2 1 1 0	EFG
2.124E+00	1.127E+02	90	D046	2 2 1 1 0	EFG

121. $C_3H_3NOS_2$

Rhodanine
Rhodanin

RN: 141-84-4 **MP** (°C)**:** 170
MW: 133.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E-02	2.250E+00	25	F300	1 0 0 0 2	

122. $C_3H_3N_3O_3$
Cyanuric acid
Cyanursaeure
Isocyanuric acid
Isocyanursaeure
RN: 108-80-5 **MP** (°C)**:**
MW: 129.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	2.969E+00	2	B193	1 2 0 0 1	
3.874E-02	5.000E+00	20	F300	1 0 0 0 0	
2.009E-02	2.593E+00	25	B384	0 0 0 0 0	

123. $C_3H_3N_3O_3$
Cyamelide
Cyamelid
RN: 462-02-2 **MP** (°C)**:**
MW: 129.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.747E-04	1.000E-01	15	F300	1 0 0 0 0	

124. $C_3H_3N_3S_3$
Trithiocyanuric acid
s-Triazine-2,4,6-trithiol
Trimercapto-*s*-triazine
RN: 638-16-4 **MP** (°C)**:**
MW: 177.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.399E-01	25	B384	0 0 0 0 0	

125. C_3H_4
Propyne
Methyl acetylene
Methylacetylene
RN: 74-99-7 **MP** (°C)**:** –101
MW: 40.07 **BP** (°C)**:** –23.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.085E-02	3.239E+00	21	I011	1 2 2 1 2	
9.085E-02	3.640E+00	25	M001	2 1 2 2 2	
5.488E-02	2.199E+00	38	I011	1 2 2 1 1	
3.606E-02	1.445E+00	54	I011	1 2 2 1 1	
2.220E-02	8.895E-01	71	I011	1 2 2 1 1	
8.886E-03	3.560E-01	88	I011	1 2 2 1 1	

126. $C_3H_4ClN_5$
Desethyl simazine
Amino-2-chloro-6-ethylamino-*s*-triazine
6-Chloro-*N*-ethyl-1,3,5-triazine-2,4-diamine
RN: 1007-28-9 **MP** (°C)**:**
MW: 145.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.747E-01	2	B193	1 1 0 0 0	

127. $C_3H_4Cl_2$
1,2-Dichloropropene
Dichloropropylene
RN: 26952-23-8 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

128. $C_3H_4Cl_2$
trans-1,3-Dichloropropene
1,3-Dichloropropylene (*trans*)
trans-1,3-Dichloropropylene
1,3-Dichloropropene
RN: 542-75-6 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.703E-03	2.999E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
9.011E-03	1.000E+00	20	M161	1 0 0 0 0	
1.071E-02	1.188E+00	30	M300	1 1 2 2 2	

129. $C_3H_4Cl_2$
cis-1,3-Dichloropropene
1,3-Dichloropropropylene (*cis*)
cis-1,3-Dichloropropylene
cis 1,3-Dichloro-propene
cis-1,3-Dichloro-1-propene
(Z)-1,3-Dichloropropene
RN: 10061-01-5 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	2.700E+00	20	G080	1 0 0 0 1	
9.651E-03	1.071E+00	30	M300	1 1 2 2 2	
8.211E-03	9.112E-01	30	M311	1 1 2 2 2	

130. $C_3H_4Cl_2$

trans-1,3-Dichloro-propene
trans-1,3-Dichloro-1-propene
(E)-1,3-Dichloro-1-propene
E-1,3-Dichloropropene

RN: 10061-02-6 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 111

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	2.800E+00	20	G080	1 0 0 0 1	

131. $C_3H_4Cl_2O_2$

Dalapon
α,α-Dichlor-propionsaeure

RN: 75-99-0 **MP** (°C)**:**
MW: 142.97 **BP** (°C)**:** 187.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E+00	5.020E+02	25	M161	1 0 0 0 2	
3.511E+00	5.020E+02	ns	K138	0 0 0 0 1	

132. $C_3H_4N_2O$

Cyanoacetamide
Cyanessigsaeure-amid

RN: 107-91-5 **MP** (°C)**:**
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E+00	1.300E+02	20	F300	1 0 0 0 1	

133. $C_3H_4N_2O_2$

Hydantoin
2,4-Imidazolidinedione

RN: 461-72-3 **MP** (°C)**:** 220
MW: 100.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E+00	2.946E+02	100	F300	1 0 0 0 2	
3.970E-01	3.973E+01	ns	M025	0 2 0 1 2	

134. $C_3H_4N_2O_3S$

2-Imidazole sulfonic acid
Imidazol-sulfosaeure-(2)
RN: 53744-47-1 **MP** (°C)**:**
MW: 148.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.009E-01	7.420E+01	20	F300	1 0 0 0 2	

135. $C_3H_4N_4O_2$

Ammelide
2,4-Dihydroxy-6-amino-1,3,5-triazine
RN: 645-93-2 **MP** (°C)**:**
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.685E-02	2	B193	1 2 0 0 0	

136. C_3H_4O

Acrolein
2-Propenal
Acrylaldehyde
RN: 107-02-8 **MP** (°C)**:** –88.0
MW: 56.06 **BP** (°C)**:** 52.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.690E+00	4.872E+02	0	B111	1 0 0 1 1	Quinol as a stabilizer
3.764E+00	2.110E+02	20	F300	1 0 0 0 2	
3.071E+00	1.722E+02	20	M161	1 0 0 0 1	
8.522E+00	4.778E+02	32.50	B111	1 0 0 1 2	Quinol as a stabilizer
8.429E+00	4.726E+02	44.40	B111	1 0 0 1 2	Quinol as a stabilizer
8.339E+00	4.675E+02	50	B111	1 0 0 1 2	Quinol as a stabilizer
8.288E+00	4.647E+02	53	B111	1 0 0 1 2	Quinol as a stabilizer
7.889E+00	4.423E+02	74.50	B111	1 0 0 1 2	Quinol as a stabilizer
7.338E+00	4.114E+02	82	B111	1 0 0 1 2	Quinol as a stabilizer
7.013E+00	3.932E+02	84	B111	1 0 0 1 2	Quinol as a stabilizer
6.597E+00	3.699E+02	87.80	B111	1 0 0 1 2	Quinol as a stabilizer
6.417E+00	3.598E+02	88	B111	1 0 0 1 2	Quinol as a stabilizer
5.096E+00	2.857E+02	ns	B185	0 0 0 0 0	
3.567E+00	2.000E+02	ns	B200	0 0 0 0 0	

137. $C_3H_4O_4$
Malonic acid
Acide malonique
Malonsaeure
RN: 141-82-2 **MP** (°C)**:** 135
MW: 104.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.645E+00	3.793E+02	0	F300	1 0 0 0 2	
5.871E+00	6.110E+02	0	L041	1 0 0 1 2	
4.990E+00	5.192E+02	0	M043	1 0 0 0 2	
5.871E+00	6.110E+02	0	M051	1 0 0 0 2	
4.743E+00	4.936E+02	4.99	A339	0 0 0 0 0	
5.427E+00	5.648E+02	10	K077	1 2 2 2 2	average of 3
5.395E+00	5.614E+02	10	M043	1 0 0 0 2	
4.888E+00	5.087E+02	9.99	A339	0 0 0 0 0	
5.034E+00	5.238E+02	14.99	A339	0 0 0 0 0	
5.608E+00	5.836E+02	15	K077	1 2 2 2 2	
6.746E+00	7.020E+02	15	L041	1 0 0 1 2	
6.746E+00	7.020E+02	15	M051	1 0 0 0 2	
5.728E+00	5.961E+02	18	K077	1 2 2 2 2	
5.198E+00	5.409E+02	19.99	A339	0 0 0 0 0	
7.063E+00	7.350E+02	20	L041	1 0 0 1 2	
5.811E+00	6.047E+02	20	M043	1 0 0 0 2	
4.067E+00	4.232E+02	20	M171	1 0 0 0 2	
2.670E+00	2.778E+02	20	S006	1 0 0 0 2	
5.928E+00	6.169E+02	24	K077	1 2 2 2 2	
5.354E+00	5.571E+02	24.99	A339	0 0 0 0 0	
4.221E+00	4.393E+02	25	F300	1 0 0 0 2	
5.990E+00	6.233E+02	25	K077	1 2 2 2 2	
7.332E+00	7.630E+02	25	M051	1 0 0 0 2	
5.494E+00	5.717E+02	29.99	A339	0 0 0 0 0	
6.178E+00	6.429E+02	30	M043	1 0 0 0 2	
5.638E+00	5.867E+02	34.99	A339	0 0 0 0 0	
7.938E+00	8.260E+02	35	L041	1 0 0 1 2	
5.800E+00	6.035E+02	39.99	A339	0 0 0 0 0	
6.530E+00	6.795E+02	40	M043	1 0 0 0 2	
5.913E+00	6.153E+02	44.99	A339	0 0 0 0 0	
6.028E+00	6.273E+02	49.99	A339	0 0 0 0 0	
8.898E+00	9.260E+02	50	L041	1 0 0 1 2	
8.898E+00	9.260E+02	50	M051	1 0 0 0 2	
6.895E+00	7.175E+02	53	K077	1 2 2 2 2	
6.182E+00	6.433E+02	54.99	A339	0 0 0 0 0	
6.328E+00	6.585E+02	59.99	A339	0 0 0 0 0	
7.158E+00	7.449E+02	60	M043	1 0 0 0 2	
6.451E+00	6.713E+02	64.99	A339	0 0 0 0 0	
9.831E+00	1.023E+03	65	L041	1 0 0 1 2	
7.878E+00	8.198E+02	80	M043	1 0 0 0 2	
8.267E+00	8.603E+02	93	K077	1 2 2 2 2	
8.554E+00	8.901E+02	100	M043	1 0 0 0 2	
9.610E+00	1.000E+03	132	K077	1 2 2 2 2	
1.441E+01	1.500E+03	ns	D072	0 0 0 0 1	

138. C_3H_5Br
Allyl bromide
3-Bromopropene
RN: 106-95-6 **MP** (°C)**:** –119
MW: 120.98 **BP** (°C)**:** 71.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.170E-02	3.835E+00	25	M342	1 0 1 1 2	

139. $C_3H_5Bvr_2Cl$
1,2-Dibromo-3-chloropropane
1-Chloro-2,3-dibromopropane
Nemagon
RN: 96-12-8 **MP** (°C)**:**
MW: 236.34 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.204E-03	1.230E+00	20	G080	1 0 0 0 1	
4.227E-03	9.990E-01	20	P081	1 0 0 0 0	
4.227E-03	9.990E-01	ns	I316	0 0 0 0 0	
4.227E-03	9.990E-01	ns	M061	0 0 0 0 0	
4.231E-03	1.000E+00	rt	M161	0 0 0 0 0	

140. C_3H_5Cl
Allyl chloride
3-Chloro-1-propene
RN: 107-05-1 **MP** (°C)**:** –134
MW: 76.53 **BP** (°C)**:** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-02	3.587E+00	20	G056	1 0 0 0 2	
1.305E-02	9.990E-01	ns	N034	0 0 0 0 0	

141. C_3H_5ClO
Chloroacetone
1-Chloro-2-propanone
Chloraceton
RN: 78-95-5 **MP** (°C)**:** –44.5
MW: 92.53 **BP** (°C)**:** 119.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.924E-01	8.257E+01	ns	N034	0 0 0 0 0	

142. C_3H_5ClO

Epichlorohydrin
Epichloridrina

RN: 106-89-8 **MP** (°C)**:** –25.6
MW: 92.53 **BP** (°C)**:** 117.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-01	6.086E+01	0	L061	1 2 2 1 2	
6.615E-01	6.121E+01	10	L061	1 2 2 1 2	
6.501E-01	6.015E+01	20	I313	0 0 0 0 0	
6.692E-01	6.191E+01	30.20	L061	1 2 2 1 2	
7.568E-01	7.003E+01	52	L061	1 2 2 1 2	
8.421E-01	7.792E+01	65	L061	1 2 2 1 2	
9.232E-01	8.542E+01	72	L061	1 2 2 1 2	
1.024E+00	9.478E+01	80.20	L061	1 2 2 1 2	

143. $C_3H_5Cl_2NO_2$

1,1-Dichloro-1-nitropropane
Propane, 1,1-dichloro-1-nitro-

RN: 595-44-8 **MP** (°C)**:**
MW: 157.98 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.149E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, *sic*

144. $C_3H_5Cl_3$

1,2,3-Trichloropropane
Allyl trichloride
Trichlorohydrin
Glycerol trichlorohydrin

RN: 96-18-4 **MP** (°C)**:** –14
MW: 147.43 **BP** (°C)**:** 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-02	1.900E+00	ns	H123	0 0 0 0 0	

145. $C_3H_5IO_2$

β-Iodopropionic acid
β-Iod-propionsaeure

RN: 141-76-4 **MP** (°C)**:** 81.5
MW: 199.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.715E-01	7.430E+01	25	F300	1 0 0 0 2	

146. C_3H_5N
Propionitrile
Propionsaeure-nitril
n-Propionitrile
RN: 107-12-0 **MP** (°C)**:** –93
MW: 55.08 **BP** (°C)**:** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.151E-02	3.388E+00	25	B004	0 0 0 0 0	

147. C_3H_5N
Ethyl isocyanide
Ethane, isocyano-
RN: 624-79-3 **MP** (°C)**:**
MW: 55.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.814E-02	9.990E-01	ns	L055	0 0 0 0 1	

148. C_3H_5NO
Acrylamide
2-Propenamide
RN: 79-06-1 **MP** (°C)**:** 84
MW: 71.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.299E+00	3.056E+02	0	M147	0 2 1 1 0	EFG
4.690E+00	3.333E+02	10	M147	0 2 1 1 0	EFG
5.220E+00	3.711E+02	20	M147	0 2 1 1 0	EFG
5.695E+00	4.048E+02	30	M147	0 2 1 1 0	EFG
6.075E+00	4.318E+02	40	M147	0 2 1 1 0	EFG
6.253E+00	4.444E+02	50	M147	0 2 1 1 0	EFG
6.625E+00	4.709E+02	60	M147	0 2 1 1 0	EFG
7.034E+00	5.000E+02	80	M147	0 2 1 1 0	EFG

149. $C_3H_5NO_3$
Formylglycine
N-Formyl glycine
RN: 2491-15-8 **MP** (°C)**:**
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E+00	1.906E+02	25	M024	1 2 0 1 2	
1.849E+00	1.906E+02	ns	M025	0 2 0 1 2	

150. $C_3H_5N_3O$
Ethylnitrosocyanamide
ENC
RN: 38434-77-4 **MP** (°C)**:**
MW: 99.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.387E+01	24	M031	1 1 1 1 1	

151. $C_3H_5N_3O_9$
Nitroglycerin
Nitroglycerol
RN: 55-63-0 **MP** (°C)**:** 13.5
MW: 227.09 **BP** (°C)**:** 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.629E-03	1.278E+00	15	L063	2 0 1 1 2	
7.926E-03	1.800E+00	20	F300	1 0 0 0 1	
6.069E-03	1.378E+00	20	L063	2 0 1 1 2	
5.504E-03	1.250E+00	25	P312	0 0 0 0 0	
6.595E-03	1.498E+00	30	L063	2 0 1 1 2	
7.342E-03	1.667E+00	40	L063	2 0 1 1 2	
8.570E-03	1.946E+00	50	L063	2 0 1 1 2	
1.041E-02	2.364E+00	60	L063	2 0 1 1 2	
1.265E-02	2.872E+00	70	L063	2 0 1 1 2	
1.518E-02	3.448E+00	80	L063	2 0 1 1 2	

152. $C_3H_5N_5O$
Ammeline
Ammelin
RN: 645-92-1 **MP** (°C)**:**
MW: 127.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.626E-02	2	B193	1 1 0 0 0	
5.901E-04	7.500E-02	23	F300	1 0 0 0 1	
2.486E-03	3.160E-01	100	F300	1 0 0 0 2	

153. C_3H_6

Cyclopropane
Trimethylene

RN: 75-19-4 **MP** (°C)**:** –127
MW: 42.08 **BP** (°C)**:** –33

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.461E-02	1.036E+00	5.05	Z008	2 1 2 2 2	at 97.26 kPa
1.281E-02	5.390E-01	20	R060	0 0 0 0 0	
1.754E-02	7.382E-01	21	I017	1 2 2 1 2	at 16.9 psia
1.103E-02	4.640E-01	25	R060	0 0 0 0 0	
9.315E-03	3.920E-01	30	R060	0 0 0 0 0	
8.983E-03	3.780E-01	31	R060	0 0 0 0 0	
7.723E-03	3.250E-01	35	R060	0 0 0 0 0	
1.083E-02	4.557E-01	38	I017	1 2 2 1 2	at 17.0 psia
6.844E-03	2.880E-01	39	R060	0 0 0 0 0	
5.917E-03	2.490E-01	45	R060	0 0 0 0 0	
8.386E-03	3.529E-01	71	I017	1 2 2 1 2	at 19.9 psia
3.999E-03	1.683E-01	104	I017	1 2 2 1 2	at 24.9 psia
5.896E+00	2.481E+02	ns	R028	0 0 0 0 0	

154. C_3H_6

Propylene
Methyl ethylene
Propene

RN: 115-07-1 **MP** (°C)**:** –185
MW: 42.08 **BP** (°C)**:** –48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.139E-02	9.000E-01	0	F300	1 0 0 0 1	
7.553E-03	3.178E-01	21	A052	1 1 1 2 2	smoothed
7.842E-03	3.300E-01	25	F300	1 0 0 0 1	
4.753E-03	2.000E-01	25	M001	2 1 2 2 2	
4.221E-03	1.776E-01	38	A052	1 1 1 2 1	smoothed
2.333E-03	9.818E-02	54	A052	1 1 1 2 1	smoothed
1.500E-03	6.312E-02	71	A052	1 1 1 2 1	smoothed
7.222E-04	3.039E-02	88	A052	1 1 1 2 1	smoothed

155. C_3H_6BrCl

1-Bromo-3-chloropropane
w-Chlorobromopropane
3-Bromopropyl chloride
3-Chloro-1-bromopropane

RN: 109-70-6 **MP** (°C)**:** –58.9
MW: 157.44 **BP** (°C)**:** 143.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-02	2.236E+00	25	M342	1 0 1 1 2	

156. $C_3H_6BrNO_4$
Bronopol
2-Bromo-2-nitropropane-1,3-diol
RN: 52-51-7 **MP** (°C)**:** 130
MW: 199.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+00	2.000E+02	22	M161	1 0 0 0 1	

157. $C_3H_6Br_2$
Trimethylene bromide
1,3-Dibromopropane
RN: 109-64-8 **MP** (°C)**:** –36
MW: 201.90 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.406E-03	1.697E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

158. $C_3H_6ClNO_2$
1-Chloro-1-nitropropane
Propane, 1-chloro-1-nitro-
RN: 600-25-9 **MP** (°C)**:**
MW: 123.54 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
4.027E-02	4.975E+00	20	M061	1 0 0 0 0	

159. $C_3H_6ClNO_2$
1-Chloro-2-nitropropane
Propane, 1-chloro-2-nitro-
RN: 37809-02-2 **MP** (°C)**:**
MW: 123.54 **BP** (°C)**:** 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	M061	1 0 0 0 0	

160. $C_3H_6Cl_2$
Propylene dichloride
1,2-Dichlor-propan
1,2-Dichloropropane
Propylene chloride
Dichloropropane
RN: 78-87-5 **MP** (°C)**:** –100.3
MW: 112.99 **BP** (°C)**:** 96.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.160E-02	3.570E+00	20	C094	1 0 1 0 2	
2.383E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
2.390E-02	2.700E+00	20	F300	1 0 0 0 1	
2.390E-02	2.700E+00	20	M037	1 1 0 0 1	
2.383E-02	2.693E+00	20	M061	1 0 0 0 1	
2.295E-02	2.593E+00	20	M062	1 0 0 0 1	
2.390E-02	2.700E+00	20	M161	1 0 0 0 1	
2.500E-02	2.825E+00	20	M312	1 0 0 0 1	
2.383E-02	2.693E+00	20	N034	1 0 0 0 1	
2.478E-02	2.800E+00	25	F300	1 0 0 0 1	
2.480E-02	2.802E+00	25	G038	1 2 2 2 2	
2.480E-02	2.802E+00	25	G053	2 1 2 1 2	
2.295E-02	2.593E+00	25	G056	1 0 0 0 2	
2.142E-02	2.420E+00	30	M300	1 1 2 2 2	
1.831E-02	2.069E+00	30	M311	1 1 2 2 2	

161. $C_3H_6Cl_2$
1,3-Dichloropropane
1,3-Dichlor-propan
RN: 142-28-9 **MP** (°C)**:** –99
MW: 112.99 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-02	2.892E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
2.416E-02	2.730E+00	25	F300	1 0 0 0 2	
2.430E-02	2.746E+00	25	G038	1 2 2 2 2	
2.430E-02	2.746E+00	25	G053	2 1 2 1 2	
9.027E-03	1.020E+00	30	M311	1 1 2 2 2	

162. $C_3H_6Cl_2O$
1,3-Dichloro-2-propanol
1,3-Dichlor-propanol-(2)
RN: 96-23-1 **MP** (°C)**:** –4
MW: 128.99 **BP** (°C)**:** 174.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.675E-01	9.900E+01	19	F300	1 0 0 0 1	
6.984E-01	9.008E+01	19	N034	1 0 0 0 1	
1.124E+00	1.450E+02	72	F300	1 0 0 0 2	

163. $C_3H_6N_2O_2$
Malonic acid diamide
Malonsaeure-diamid
Malonamide
Malonodiamide
Propanediamide
RN: 108-13-4 **MP** (°C)**:** 170
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.513E-01	7.670E+01	8	F300	1 0 0 0 2	
7.830E-03	7.994E-01	ns	L055	0 0 0 0 1	

164. $C_3H_6N_2O_2$
Methylglyoxime
Methylglyoxim
RN: 1804-15-5 **MP** (°C)**:**
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-01	4.600E+01	26	F300	1 0 0 0 1	
7.444E-01	7.600E+01	40	F300	1 0 0 0 1	

165. $C_3H_6N_2O_2$
Methylnitrosoacetamide
MNA
RN: 7417-67-6 **MP** (°C)**:**
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-01	1.736E+01	24	M031	1 1 1 1 1	

166. $C_3H_6N_2O_2$
1-Acetylurea
Acetylharnstoff
RN: 591-07-1 **MP** (°C)**:** 218
MW: 102.09 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-01	1.300E+01	15	F300	1 0 0 0 1	

167. $C_3H_6N_2O_3$
Hydantoic acid
N-(Carboxymethyl)urea
N-Carbamoylglycine
Carbamoylglycine
Glycoluric acid
RN: 462-60-2 **MP** (°C)**:**
MW: 118.09 **BP** (°C)**:**

Solub ility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E-01	3.010E+01	20	F300	1 0 0 0 2	
3.290E-01	3.885E+01	25	M024	1 2 0 1 2	
3.290E-01	3.885E+01	ns	M025	0 2 0 1 2	

168. $C_3H_6N_2O_7$
Glycerol 1,2-dinitrate
1,2,3-Propanetriol 1,2-dinitrate
1,2-Dinitroglycerol
RN: 131287-51-9 **MP** (°C)**:**
MW: 182.09 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.386E-01	6.165E+01	20	D013	1 0 1 1 2	

169. $C_3H_6N_2O_7$
Glycerol 1,3-dinitrate
Glycerol-α,α′-dinitrate
Glycerin-α,α′-dinitrate
RN: 623-87-0 **MP** (°C)**:** 26
MW: 182.09 **BP** (°C)**:** 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.993E-01	7.270E+01	20	D013	1 0 1 1 2	

170. $C_3H_6N_2S$
Ethylenethiourea
Mercaptoimidazoline
Mercozen
RN: 96-45-7 **MP** (°C)**:** 203
MW: 102.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-01	1.961E+01	30	I310	0 0 0 0 0	
8.082E-01	8.257E+01	60	I310	0 0 0 0 0	
2.991E+00	3.056E+02	90	I310	0 0 0 0 0	

171. $C_3H_6N_4Hg$

Methylmercuridicyanodiamide
Panogen

RN: 502-39-6 **MP** (°C)**:** 156
MW: 298.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.265E-02	2.170E+01	20	M061	1 0 0 0 2	
7.265E-02	2.170E+01	rt	M161	0 0 0 0 2	

172. $C_3H_6N_6$

Melamine
1,3,5-Triazine-2,4,6-triamine
Cymel

RN: 108-78-1 **MP** (°C)**:**
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.503E-03	1.199E+00	0	M043	1 0 0 0 1	
1.000E-02	1.261E+00	2	B193	1 1 0 0 1	
1.425E-02	1.797E+00	10	M043	1 0 0 0 1	
2.561E-02	3.230E+00	19.90	C023	2 2 0 1 2	
2.135E-02	2.693E+00	20	M043	1 0 0 0 1	
3.316E-02	4.182E+00	30	M043	1 0 0 0 1	
4.651E-02	5.865E+00	34.90	C023	2 2 0 1 2	
5.590E-02	7.050E+00	40	M043	1 0 0 0 1	
8.200E-02	1.034E+01	49.80	C023	2 2 0 1 2	
1.172E-01	1.478E+01	60	M043	1 0 0 0 1	
1.325E-01	1.672E+01	64.10	C023	2 2 0 1 2	
1.836E-01	2.315E+01	74.50	C023	2 2 0 1 2	
2.160E-01	2.724E+01	80	M043	1 0 0 0 1	
2.421E-01	3.054E+01	83.50	C023	2 2 0 1 2	
3.480E-01	4.389E+01	94.80	C023	2 2 0 1 2	
3.812E-01	4.807E+01	99	C023	2 2 0 1 2	
3.776E-01	4.762E+01	100	M043	1 0 0 0 1	

173. $C_3H_6N_6O_6$

Cyclonite
RDX

RN: 121-82-4 **MP** (°C)**:** 205
MW: 222.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	5.975E-02	25	B173	2 0 2 2 2	

174. C_3H_6O

Propylene oxide
Methyl ethylene oxide

RN: 75-56-9 **MP** (°C)**:** –112
MW: 58.08 **BP** (°C)**:** 34.23

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E+00	2.883E+02	20	I313	0 0 0 0 0	
2.544E-01	1.478E+01	20	M065	1 0 2 1 1	*sic*
6.389E+00	3.711E+02	25	I313	0 0 0 0 0	

175. C_3H_6O

Acetone
2-Propanone
Aceton

RN: 67-64-1 **MP** (°C)**:** –94
MW: 58.08 **BP** (°C)**:** 56.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
		4	C423	0 0 0 0 0	
		10	C423	0 0 0 0 0	

176. C_3H_6O

Propaldehyde
Propyl aldehyde
Propanal

RN: 123-38-6 **MP** (°C)**:** –81
MW: 58.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E+00	1.667E+02	20	D041	1 0 0 0 0	
2.927E+00	1.700E+02	20	F300	1 0 0 0 1	
5.269E+00	3.060E+02	25	A049	1 0 0 0 2	
3.105E+00	1.803E+02	25	B060	2 0 1 1 1	
2.880E+00	1.673E+02	25	F044	1 0 0 0 2	

177. $C_3H_6O_2$

Propionic acid
n-Propionic acid

RN: 79-09-4 **MP** (°C)**:** –22
MW: 74.08 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.025E+01	25	B004	0 0 0 0 0	

178. $C_3H_6O_2$

Ethyl formate
Ameisensaeure-aethyl ester
Formic acid ethyl ester

RN: 109-94-4 **MP** (°C)**:** –80
MW: 74.08 **BP** (°C)**:** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.094E+00	8.108E+01	5.0	K079	1 0 0 0 2	
1.139E+00	8.437E+01	15.9	K079	1 0 0 0 2	
1.350E+00	1.000E+02	18	F300	1 0 0 0 1	
1.350E+00	1.000E+02	22	S006	1 0 0 0 2	
1.194E+00	8.848E+01	30.2	K079	1 0 0 0 2	
1.239E+00	9.178E+01	38.0	K079	1 0 0 0 2	
1.283E+00	9.507E+01	45.1	K079	1 0 0 0 2	
1.339E+00	9.918E+01	50.0	K079	1 0 0 0 2	
1.383E+00	1.025E+02	55.5	K079	1 0 0 0 2	
1.517E+00	1.124E+02	63.9	K079	1 0 0 0 2	
1.639E+00	1.214E+02	70.0	K079	1 0 0 0 2	
1.778E+00	1.317E+02	75.5	K079	1 0 0 0 2	

179. $C_3H_6O_2$

Methyl acetate
Essigsaeures methyl
Methylacetat

RN: 79-20-9 **MP** (°C)**:** –98.0
MW: 74.08 **BP** (°C)**:** 56.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.678E+00	2.725E+02	5.0	K079	1 0 0 0 2	
4.017E+00	2.976E+02	20	E002	1 0 0 0 2	
3.290E+00	2.437E+02	20	F001	1 0 1 2 2	
2.647E+00	1.961E+02	20	F300	1 0 0 0 2	
3.290E+00	2.437E+02	20	M171	1 0 0 0 2	
4.617E+00	3.420E+02	20	P040	0 0 0 0 0	
4.300E+00	3.185E+02	20	S006	1 0 0 0 1	
3.722E+00	2.757E+02	21.0	K079	1 0 0 0 2	
2.772E-02	2.054E+00	25	B004	0 0 0 0 0	*sic*
3.772E+00	2.794E+02	35.0	K079	1 0 0 0 2	
3.889E+00	2.881E+02	58.0	K079	1 0 0 0 2	
3.906E+00	2.893E+02	58.9	K079	1 0 0 0 2	
3.922E+00	2.906E+02	60.1	K079	1 0 0 0 2	
3.950E+00	2.926E+02	61.7	K079	1 0 0 0 2	
4.172E+00	3.091E+02	69.1	K079	1 0 0 0 2	
4.256E+00	3.153E+02	70.5	K079	1 0 0 0 2	
4.294E+00	3.181E+02	71.9	K079	1 0 0 0 2	
4.906E+00	3.634E+02	83.5	K079	1 0 0 0 2	
4.252E-02	3.150E+00	c	L055	0 0 0 0 2	

180. $C_3H_6O_2S_3$
α-Trimethylene trisulphide dioxide
1,3,5-Trithiane, 1,3-dioxide, *trans*-
RN: 60077-04-5 **MP** (°C)**:**
MW: 170.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.817E-02	1.672E+01	25	B112	1 2 1 1 2	

181. $C_3H_6O_2S_3$
β-Trimethylene trisulphide dioxide
1,3,5-Trithiane, 1,3-dioxide, *cis*-
RN: 60041-48-7 **MP** (°C)**:**
MW: 170.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.545E-01	4.334E+01	25	B112	1 2 1 1 2	

182. $C_3H_6O_3$
DL-Glyceraldehyde
DL-Glycerin-aldehyd
RN: 56-82-6 **MP** (°C)**:** 145
MW: 90.08 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E-01	2.913E+01	18	D041	1 0 0 0 0	
3.242E-01	2.920E+01	18	F300	1 0 0 0 2	

183. $C_3H_6O_3$
Hydracrylic acid
Hydracrylsaeure
RN: 503-66-2 **MP** (°C)**:**
MW: 90.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.998E+00	2.701E+02	25	I307	0 0 0 0 0	

184. $C_3H_6O_3$
s-Trioxane
1,3,5-Trioxan
RN: 110-88-3 **MP** (°C)**:** 64
MW: 90.08 **BP** (°C)**:** 114.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E+00	1.544E+02	20.00	B394	0 0 0 0 0	
1.943E+00	1.750E+02	25	F300	1 0 0 0 2	
2.033E+00	1.831E+02	25.00	B394	0 0 0 0 0	
2.403E+00	2.165E+02	30.10	B394	0 0 0 0 0	
2.741E+00	2.469E+02	34.45	B394	0 0 0 0 0	
4.187E+00	3.772E+02	43.00	B394	0 0 0 0 0	
4.462E+00	4.019E+02	44.00	B394	0 0 0 0 0	
4.606E+00	4.149E+02	44.40	B394	0 0 0 0 0	
4.826E+00	4.348E+02	45.00	B394	0 0 0 0 0	
4.816E+00	4.338E+02	45.10	B394	0 0 0 0 0	
5.355E+00	4.824E+02	46.00	B394	0 0 0 0 0	
5.311E+00	4.784E+02	46.10	B394	0 0 0 0 0	
6.401E+00	5.766E+02	47.10	B394	0 0 0 0 0	
8.161E+00	7.351E+02	47.80	B394	0 0 0 0 0	
8.534E+00	7.687E+02	48.95	B394	0 0 0 0 0	
8.741E+00	7.874E+02	50.20	B394	0 0 0 0 0	
9.095E+00	8.192E+02	55.30	B394	0 0 0 0 0	

185. $C_3H_6O_3S_3$
α-Trimethylene trisulphoxide
1,3,5-Trithiane, 1,3,5-trioxide, (1α,3α,5α)-
RN: 60102-87-6 **MP** (°C)**:**
MW: 186.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.184E-03	1.338E+00	25	B112	1 2 1 1 2	

186. $C_3H_6O_3S_3$
β-Trimethylene trisulphoxide
1,3,5-Trithiane, 1,3,5-trioxide, (1α,3α,5β)-
RN: 60102-88-7 **MP** (°C)**:**
MW: 186.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-02	1.417E+01	25	B112	1 2 1 1 2	

187. $C_3H_6O_3S$
1,3-Propane sultone
1,2-Oxathiolane 2,2-dioxide
3-Hydroxy-1-propanesulfonic acid g-sultone
RN: 1120-71-4 **MP** (°C)**:** 31
MW: 122.14 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.187E-01	1.000E+02	ns	I307	0 0 0 0 0	

188. C_3H_7Br
Isopropyl bromide
Isopropylbromid
RN: 75-26-3 **MP** (°C)**:** –89
MW: 123.00 **BP** (°C)**:** 59

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-02	4.180E+00	0	H101	2 0 0 0 2	
2.340E-02	2.878E+00	18	F001	1 0 1 2 2	
2.602E-02	3.200E+00	20	F300	1 0 0 0 1	
2.585E-02	3.180E+00	20	H101	2 0 0 0 2	
2.592E-02	3.188E+00	30	V009	1 0 0 0 1	

189. C_3H_7Br
Propyl bromide
1-Bromopropane
Propylbromid
Bromopropane
RN: 106-94-5 **MP** (°C)**:** –110
MW: 123.00 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-02	2.970E+00	0	F300	1 0 0 0 2	
2.423E-02	2.980E+00	0	H101	2 0 0 0 2	
1.850E-02	2.275E+00	19.5	S006	1 0 0 0 2	
1.850E-02	2.275E+00	19.50	F001	1 0 1 0 2	
1.992E-02	2.450E+00	20	H101	2 0 0 0 2	
1.947E-02	2.394E+00	20	H127	1 0 0 0 1	
1.874E-02	2.305E+00	30	G029	1 0 2 2 2	
1.876E-02	2.307E+00	30	V009	1 0 0 0 2	
1.140E-01	1.402E+01	ns	H307	0 0 0 0 0	

190. C_3H_7BrO
3-Bromo-1-propanol
3-Brom-propanol-(1)
RN: 627-18-9 **MP** (°C)**:**
MW: 139.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.022E+00	1.420E+02	20	F300	1 0 0 0 2	

191. C_3H_7Cl
Isopropyl chloride
2-Chloropropane
RN: 75-29-6 **MP** (°C)**:** –117
MW: 78.54 **BP** (°C)**:** 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.602E-02	4.400E+00	0	H101	2 0 0 0 2	
4.380E-02	3.440E+00	12.50	F001	1 0 1 0 2	
3.947E-02	3.100E+00	20	F300	1 0 0 0 1	
3.883E-02	3.050E+00	20	H101	2 0 0 0 2	
3.935E-02	3.090E+00	20	N034	1 0 0 0 1	
3.888E-02	3.054E+00	30	V009	1 0 0 0 1	

192. C_3H_7Cl
Chloropropane
Propyl chloride
1-Chloropropane
RN: 540-54-5 **MP** (°C)**:** –123
MW: 78.54 **BP** (°C)**:** 43.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.787E-02	3.760E+00	0	H101	2 0 0 0 2	
2.970E-02	2.333E+00	12.50	F001	1 0 1 0 2	
3.438E-02	2.700E+00	20	F300	1 0 0 0 1	
3.463E-02	2.720E+00	20	H101	2 0 0 0 2	
3.428E-02	2.693E+00	20	N034	1 0 0 0 1	
2.970E-02	2.333E+00	20	S006	1 0 0 0 2	
3.520E-02	2.765E+00	30	V009	1 0 0 0 2	

193. C_3H_7ClO

3-Chloro-1-propanol
3-Chlor-propanol-(1)
RN: 627-30-5 **MP** (°C)**:**
MW: 94.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E+00	2.500E+02	20	F300	1 0 0 0 1	
+2.64E+00	+2.50E+02	ns	S460	0 0 0 0 0	

194. C_3H_7I

Iodopropane
n-Propyl iodide
RN: 107-08-4 **MP** (°C)**:** –101
MW: 169.99 **BP** (°C)**:** 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-03	1.140E+00	0	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	F001	1 0 1 0 2	
5.118E-03	8.700E-01	20	F300	1 0 0 0 1	
6.294E-03	1.070E+00	20	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	M171	1 0 0 0 1	
5.100E-03	8.670E-01	20	S006	1 0 0 0 1	
6.258E-03	1.064E+00	23.5	S171	2 1 2 2 2	
6.112E-03	1.039E+00	30	G029	1 0 2 2 2	
6.094E-03	1.036E+00	30	V009	1 0 0 0 1	

195. C_3H_7I

Isopropyl iodide
2-Iodopropane
RN: 75-30-9 **MP** (°C)**:** –90
MW: 169.99 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.824E-03	1.670E+00	0	H101	2 0 0 0 2	
8.236E-03	1.400E+00	20	F300	1 0 0 0 1	
8.236E-03	1.400E+00	20	H101	2 0 0 0 2	
7.889E-03	1.341E+00	30	V009	1 0 0 0 1	

196. $C_3H_7NO_2$

1-Nitropropane
n-Nitropropane

RN: 108-03-2 **MP** (°C)**:** –108
MW: 89.09 **BP** (°C)**:** 131.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-01	1.381E+01	20	C121	1 0 0 0 1	unit assumed, *sic*

197. $C_3H_7NO_2$

2-Nitropropane
Nitroisopropane
Dimethylnitromethane

RN: 79-46-9 **MP** (°C)**:** –93
MW: 89.09 **BP** (°C)**:** 120.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-01	1.672E+01	20	C121	0 0 0 0 1	unit assumed, *sic*
1.874E-01	1.670E+01	20	F300	1 0 0 0 2	
2.376E-01	2.117E+01	20	H118	1 1 1 1 2	

198. $C_3H_7NO_2$

α-Alanine
Alanine
2-Aminopropanoic acid
2-Ammoniopropanoate
L-2-Aminopropionic acid

RN: 56-41-7 **MP** (°C)**:** 314.5–316.5
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E+00	1.217E+02	10	C347	0 0 0 0 0	EFG
1.640E+00	1.461E+02	15	D349	2 1 1 2 2	
1.744E+00	1.554E+02	20	B032	1 2 2 1 2	
1.535E+00	1.367E+02	20	C347	0 0 0 0 0	EFG
1.780E+00	1.586E+02	20	D349	2 1 1 2 2	
1.838E+00	1.638E+02	25	B032	1 2 2 1 2	
1.590E+00	1.417E+02	25	D005	2 2 1 1 2	
1.602E+00	1.427E+02	25	D041	1 0 0 0 2	
1.870E+00	1.666E+02	25	D349	2 1 1 2 2	
1.660E+00	1.479E+02	25	E015	1 2 1 1 1	
1.595E+00	1.421E+02	25	G092	2 1 1 1 1	
1.595E+00	1.421E+02	25	G315	0 0 0 0 0	
1.654E+00	1.474E+02	25	G433	0 0 0 0 0	
1.852E+00	1.650E+02	25	J303	0 0 0 0 0	
1.600E+00	1.426E+02	25	N001	0 0 0 0 0	EFG
1.630E+00	1.452E+02	25	N012	2 0 2 1 2	
1.555E+00	1.386E+02	25	O316	1 0 1 2 2	

(*continued*)

198. $C_3H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.598E+00	1.424E+02	25	O316	1 0 1 2 2	
1.623E+00	1.446E+02	25	O317	1 0 1 2 2	
1.871E+00	1.667E+02	25.1	N024	0 0 0 0 0	
1.871E+00	1.667E+02	25.1	N026	0 0 0 0 0	
1.606E+00	1.431E+02	25.1	N027	1 1 2 2 2	
1.704E+00	1.518E+02	27	D036	0 0 0 0 0	
1.695E+00	1.510E+02	27	D036	0 0 0 0 0	
1.940E+00	1.728E+02	29.80	B032	1 2 2 1 2	
1.657E+00	1.477E+02	30	C347	0 0 0 0 0	EFG
1.956E+00	1.743E+02	30	J303	0 0 0 0 0	
1.816E+00	1.618E+02	40	C347	0 0 0 0 0	EFG
2.192E+00	1.953E+02	40	J303	0 0 0 0 0	
1.931E+00	1.720E+02	45	F300	1 0 0 0 2	
1.932E+00	1.721E+02	50	C347	0 0 0 0 0	EFG
2.430E+00	2.165E+02	50	J303	0 0 0 0 0	
2.118E+00	1.887E+02	60	C347	0 0 0 0 0	EFG
2.706E+00	2.411E+02	60	J303	0 0 0 0 0	
2.333E+00	2.078E+02	70	C347	0 0 0 0 0	EFG
2.489E+00	2.218E+02	75	D041	1 0 0 0 2	
2.504E+00	2.230E+02	80	C347	0 0 0 0 0	EFG
2.668E+00	2.377E+02	90	C347	0 0 0 0 0	EFG
2.888E+00	2.573E+02	100	C347	0 0 0 0 0	EFG
1.192E+00	1.062E+02	-	C347	0 0 0 0 0	EFG
1.587E+00	1.414E+02	rt	D021	0 0 1 1 2	

199. $C_3H_7NO_2$

β-Alanine
β-Alanin
RN: 107-95-9 **MP** (°C)**:**
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E+00	3.528E+02	25	D041	1 0 0 0 2	
6.123E+00	5.455E+02	25	M024	1 2 0 1 2	

200. $C_3H_7NO_2$

D-Alanine
D(–)-Alanine
RN: 338-69-2 **MP** (°C)**:** 292
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E+00	1.127E+02	0	M043	1 0 0 0 2	
1.396E+00	1.243E+02	10	M043	1 0 0 0 2	

(*continued*)

200. $C_3H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E+00	1.363E+02	20	D041	1 0 0 0 2	
1.531E+00	1.364E+02	20	M043	1 0 0 0 2	
1.589E+00	1.416E+02	25	D005	2 2 1 1 2	
1.680E+00	1.497E+02	30	M043	1 0 0 0 2	
1.839E+00	1.639E+02	40	M043	1 0 0 0 2	
2.194E+00	1.955E+02	60	M043	1 0 0 0 2	
2.590E+00	2.308E+02	80	M043	1 0 0 0 2	
3.049E+00	2.717E+02	100	M043	1 0 0 0 2	
3.049E+00	2.717E+02	99.99	P349	0 0 0 0 0	

201. $C_3H_7NO_2$

DL-Alanine
DL-α-Alanine
DL-2-Aminopropionic acid

RN: 302-72-7 **MP** (°C)**:** 289
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	1.080E+02	0	D018	2 2 2 1 2	
1.212E+00	1.080E+02	0	F300	1 0 0 0 2	
1.212E+00	1.079E+02	0	M043	1 0 0 0 2	
1.361E+00	1.213E+02	10	M043	1 0 0 0 0	
1.523E+00	1.357E+02	20	M043	1 0 0 0 0	
1.557E+00	1.387E+02	21	P045	1 0 2 1 2	
1.659E+00	1.478E+02	25	C018	0 0 0 0 0	
1.596E+00	1.422E+02	25	D018	2 2 2 1 2	
1.598E+00	1.424E+02	25	D041	1 0 0 0 2	
1.607E+00	1.432E+02	25	F300	1 0 0 0 2	
1.900E+00	1.693E+02	25	J303	0 0 0 0 0	
1.530E+00	1.363E+02	25	K031	2 1 2 1 2	
2.024E+00	1.803E+02	30	J303	0 0 0 0 0	
1.704E+00	1.518E+02	30	M043	1 0 0 0 0	
2.307E+00	2.055E+02	40	J303	0 0 0 0 0	
1.894E+00	1.687E+02	40	M043	1 0 0 0 0	
2.134E+00	1.902E+02	50	D018	2 2 2 1 2	
2.106E+00	1.876E+02	50	F300	1 0 0 0 2	
2.591E+00	2.308E+02	50	J303	0 0 0 0 0	
2.954E+00	2.632E+02	60	J303	0 0 0 0 0	
2.337E+00	2.082E+02	60	M043	1 0 0 0 0	
2.733E+00	2.435E+02	75	D018	2 2 2 1 2	
2.734E+00	2.436E+02	75	D041	1 0 0 0 2	
2.714E+00	2.418E+02	75	F300	1 0 0 0 2	
2.842E+00	2.532E+02	80	M043	1 0 0 0 0	
3.431E+00	3.057E+02	100	F300	1 0 0 0 2	
3.430E+00	3.056E+02	100	M043	1 0 0 0 2	
3.432E+00	3.057E+02	99.99	P349	0 0 0 0 0	

202. $C_3H_7NO_2$
Lactamide
2-Hydroxypropionamide
RN: 2043-43-8 **MP** (°C)**:**
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.779E+00	7.822E+02	25	M008	1 0 0 0 2	

203. $C_3H_7NO_2$
Sarcosine
Sarkosin
RN: 107-97-1 **MP** (°C)**:** 208
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.151E-01	4.589E+01	20	D041	1 0 0 0 2	
3.367E+00	3.000E+02	20	F300	1 0 0 0 2	
4.807E+00	4.282E+02	20	P045	1 0 2 1 2	

204. $C_3H_7NO_2$
Urethan
Carbamidsaeure-aethyl ester
Eythyl urethan
Urethane
Ethyl carbamate
Carbamic acid ethyl ester
RN: 51-79-6 **MP** (°C)**:** 49
MW: 89.09 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E+00	2.600E+02	11	F300	1 0 0 0 1	
5.393E+00	4.805E+02	15.5	F001	1 0 1 2 2	
2.245E+01	2.000E+03	25	I310	0 0 0 0 0	
5.074E+00	4.521E+02	25	P065	2 0 1 1 2	
1.800E+01	1.604E+03	37	H006	1 2 2 1 1	
8.901E+00	7.930E+02	40	F300	1 0 0 0 2	

205. $C_3H_7NO_2S$
Cysteine
2-Amino-3-mercaptopropanoic acid
RN: 3374-22-9 **MP** (°C)**:** 225
MW: 121.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.773E-02	3.360E+00	20	P045	1 0 2 1 2	

206. $C_3H_7NO_3$
Serine
2-Amino-3-hydroxypropanoic acid
L(–)-Serin
RN: 56-45-1 **MP** (°C)**:** 220
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.556E+00	1.635E+02	10.19	J417	0 0 0 0 0	
1.626E+00	1.709E+02	12.69	J417	0 0 0 0 0	
4.530E-01	4.761E+01	15	D349	2 1 1 2 2	
1.864E+00	1.959E+02	16.09	J417	0 0 0 0 0	
1.903E+00	2.000E+02	20	D041	1 0 0 0 1	
4.610E-01	4.845E+01	20	D349	2 1 1 2 2	
9.512E-01	9.997E+01	20	F300	1 0 0 0 2	
3.405E+00	3.578E+02	20.00	B032	1 2 2 1 2	*sic*
4.700E-01	4.939E+01	25	D349	2 1 1 2 2	
2.807E+00	2.950E+02	25	G315	0 0 0 0 0	*sic*
4.013E+00	4.217E+02	25	J303	0 0 0 0 0	
4.043E+00	4.249E+02	25.00	B032	1 2 2 0 2	*sic*
2.228E+00	2.342E+02	25.89	J417	0 0 0 0 0	
3.578E+00	3.760E+02	27	D036	0 0 0 0 0	
2.287E+00	2.404E+02	27.89	J417	0 0 0 0 0	
4.690E+00	4.929E+02	29.80	B032	1 2 2 1 2	*sic*
5.633E+00	5.920E+02	40	J303	0 0 0 0 0	
2.800E+00	2.943E+02	42.79	J417	0 0 0 0 0	
2.811E+00	2.954E+02	43.79	J417	0 0 0 0 0	
2.861E+00	3.007E+02	44.59	J417	0 0 0 0 0	
2.902E+00	3.050E+02	49.69	J417	0 0 0 0 0	
2.972E+00	3.124E+02	53.89	J417	0 0 0 0 0	
7.574E+00	7.960E+02	60	J303	0 0 0 0 0	

207. $C_3H_7NO_3$
D-Serine
D-2-Amino-3-hydroxypropanoic acid
RN: 312-84-5 **MP** (°C)**:** 220
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.903E+00	2.000E+02	20	D041	1 0 0 0 0	
4.010E+00	4.214E+02	25	J303	0 0 0 0 0	
5.709E+00	6.000E+02	40	J303	0 0 0 0 0	
7.631E+00	8.020E+02	60	J303	0 0 0 0 0	

208. $C_3H_7NO_3$

DL-Serine
DL-2-Amino-3-hydroxypropanoic acid
RN: 302-84-1 **MP** (°C)**:** 240
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-01	2.920E+01	10	F300	1 0 0 0 2	
3.787E-01	3.980E+01	20	F300	1 0 0 0 2	
4.548E-01	4.780E+01	25	D041	1 0 0 0 2	
4.805E-01	5.050E+01	25	J303	0 0 0 0 0	
7.403E-01	7.780E+01	40	J303	0 0 0 0 0	
8.916E-01	9.370E+01	50	F300	1 0 0 0 2	
1.261E+00	1.325E+02	60	J303	0 0 0 0 0	
1.533E+00	1.611E+02	75	D041	1 0 0 0 2	
1.532E+00	1.610E+02	75	F300	1 0 0 0 2	
2.320E+00	2.438E+02	100	F300	1 0 0 0 2	
2.320E+00	2.438E+02	99.99	P349	0 0 0 0 0	

209. $C_3H_7NO_3$

DL-Isoserine
DL-Isoserin
RN: 632-12-2 **MP** (°C)**:** 235
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	1.530E+01	20	F300	1 0 0 0 2	

210. $C_3H_7NO_5$

Glycerol-α-nitrate
Glycerin-α-nitrate
RN: 27321-61-5 **MP** (°C)**:**
MW: 137.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E+00	4.118E+02	15	F300	1 0 0 0 2	

211. $C_3H_7N_3O_2$

Glycocyamine
Guanidin-essigsaeure
Guanidineacetic acid
RN: 352-97-6 **MP** (°C)**:** 280
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-02	4.480E+00	15	D041	1 0 0 0 1	
3.074E-02	3.600E+00	15	F300	1 0 0 0 1	

212. $C_3H_7N_3O_2$
Nitrosoethylurea
N-Nitroso-*N*-ethylurea
RN: 759-73-9 **MP** (°C)**:** 103
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	1.283E+01	rt	I306	0 0 0 0 0	

213. $C_3H_7O_5P$
2-Carboxyethylphosphonic acid
3-Phosphonopropionic acid
RN: 5962-42-5 **MP** (°C)**:**
MW: 154.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	2.842E+02	0	N028	1 0 0 0 2	
2.129E+00	3.280E+02	20	N028	1 0 0 0 2	

214. C_3H_8
Propane
Propan
RN: 74-98-6 **MP** (°C)**:** –187
MW: 44.10 **BP** (°C)**:** –42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.460E-03	1.526E-01	4	K031	2 1 2 1 2	
2.472E-03	1.090E-01	10	F300	1 0 0 0 2	
2.721E-03	1.200E-01	18	M065	0 0 2 1 1	1 atm, *sic*
1.761E-03	7.765E-02	19.8	G058	1 0 0 0 2	
1.746E-03	7.700E-02	20	F300	1 0 0 0 1	
1.420E-03	6.261E-02	25	B342	1 2 1 1 1	
1.530E-03	6.747E-02	25	K031	2 1 2 1 2	
1.415E-03	6.240E-02	25	M001	2 1 2 2 2	
1.415E-03	6.240E-02	25	M002	2 1 2 2 2	
8.400E-04	3.704E-02	50	K031	2 1 2 1 2	
6.123E-04	2.700E-02	60	F300	1 0 0 0 1	

215. $C_3H_8NO_5P$

Glyphosate
N-(Phosphonomethyl)glycine
Bronco
RN: 1071-83-6 **MP** (°C)**:** 230.0
MW: 169.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.097E-02	1.200E+01	25	M161	1 0 0 0 1	
5.856E-02	9.901E+00	ns	B100	0 0 0 0 0	

216. C_3H_8O

n-Propyl alcohol
Propanol
RN: 71-23-8 **MP** (°C)**:** –127.0
MW: 60.10 **BP** (°C)**:** 97.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E+00	1.882E+02	ns	L003	0 0 2 1 2	
+4.17E+00	+2.51E+02	ns	S460	0 0 0 0 0	

217. C_3H_8O

Isopropyl alcohol
2-Propanol
RN: 67-63-0 **MP** (°C)**:** –88
MW: 60.10 **BP** (°C)**:** 82.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.033E+00	3.025E+02	ns	L003	0 0 2 1 1	

218. $C_3H_8OS_2$

2,3-Dimercapto-1-propanol
Dimercaprol
RN: 59-52-9 **MP** (°C)**:**
MW: 124.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.963E-01	7.407E+01	20	D041	1 0 0 0 0	

219. $C_3H_8O_2$
Methylal
Formaldehyd-dimethyl-acetal
RN: 109-87-5 **MP** (°C)**:** –105
MW: 76.10 **BP** (°C)**:** 41.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E+00	2.441E+02	16	B117	1 0 0 1 2	
3.022E+00	2.300E+02	20	F300	1 0 0 0 1	

220. $C_3H_8O_3$
Glycerol
Glycerin
RN: 56-81-5 **MP** (°C)**:** 20
MW: 92.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.973E+00	5.501E+02	4.50	C022	1 2 0 0 2	
5.751E-01	5.296E+01	25	B004	0 0 0 0 0	

221. C_3H_9N
Propylamine
Propylamin
n-Propylamine
RN: 107-10-8 **MP** (°C)**:** –83
MW: 59.11 **BP** (°C)**:** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	1.459E+00	25	B004	0 0 0 0 0	

222. C_3H_9N
Trimethylamine
N,*N*-Dimethylmethanamine
RN: 75-50-3 **MP** (°C)**:** –124.0
MW: 59.11 **BP** (°C)**:** 3.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.77E+00	>4.00E+02	20	F300	1 0 0 0 0	
6.936E+00	4.100E+02	25	A049	1 0 0 0 2	

223. $C_3H_9O_4P$
Trimethyl phosphate
Phosphorsaeure-trimethyl ester
RN: 512-56-1 **MP** (°C)**:**
MW: 140.08 **BP** (°C)**:** 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E+00	5.000E+02	25	F300	1 0 0 0 1	
3.573E+00	5.005E+02	ns	S460	0 0 0 0 0	

224. $C_3H_{12}N_6O_3$
Guanidine carbonate
Guanidin-carbonat
RN: 3425-08-9 **MP** (°C)**:** 198
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E+00	3.333E+02	24	F300	1 0 0 0 2	

225. $C_3Cl_3N_3O_3$
Trichloroisocyanuric acid
Symclosene
RN: 87-90-1 **MP** (°C)**:** 246.5
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.439E-03	7.994E-01	20	B080	1 0 1 1 0	
2.311E-02	5.371E+00	40	B080	1 0 1 1 1	

226. C_3Cl_6
Hexachloropropene
Hexachloropropylene
Perchloropropene
Hexachloro-1-propene
1,1,2,3,3,3-Hexachloro-1-propene
1,1,2,3,3,3-Hexachloropropene
RN: 1888-71-7 **MP** (°C)**:**
MW: 248.75 **BP** (°C)**:** 209–210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.026E-04	1.499E-01	ns	S460	0 0 0 0 0	

227. C_4HI_4N
Iodol
2,3,4,5-Tetraiodpyrrol
RN: 87-58-1 **MP** (°C)**:**
MW: 570.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.505E-04	2.000E-01	15	F300	1 0 0 0 2	

228. C_4H_2
Butadiyne
Diacetylen
RN: 460-12-8 **MP** (°C)**:** –36.4
MW: 50.06 **BP** (°C)**:** 10.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	1.000E-01	25	F300	1 0 0 0 0	

229. $C_4H_2N_2O_4$
Alloxan
Alloxane
RN: 50-71-5 **MP** (°C)**:** 256dec
MW: 142.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.631E-02	8.000E+00	ns	D072	0 0 0 0 0	
5.623E-02	7.989E+00	ns	R424	0 0 0 0 0	

230. $C_4H_3BrN_2O_2$
5-Bromouracil
5-Bromo-2
4(1H,3H)-Pyrimidinedione
5-Bromo-2,4-dihydroxypyrimidine
Bromouracil
RN: 51-20-7 **MP** (°C)**:** 310
MW: 190.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.507E-02	2.878E+00	25	S471	0 0 0 0 0	
1.908E-02	3.644E+00	25	S471	0 0 0 0 0	
1.350E-02	2.578E+00	25	Z408	0 0 0 0 0	

231. $C_4H_3ClN_2O_2$

6-Chlorouracil
4-Chloro-2,6-dihydroxypyrimidine
RN: 4270-27-3 **MP** (°C)**:**
MW: 146.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.334E-02	4.885E+00	25	S471	0 0 0 0 0	
3.350E-02	4.909E+00	25	S471	0 0 0 0 0	

232. $C_4H_3ClN_2O_2$

5-Chlorouracil
RN: 1820-81-1 **MP** (°C)**:**
MW: 146.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.707E-02	2.501E+00	25	S471	0 0 0 0 0	
1.712E-02	2.509E+00	25	S471	0 0 0 0 0	
1.800E-02	2.638E+00	25	Z408	0 0 0 0 0	
9.827E-04	1.440E-01	ns	Y414	0 0 0 0 0	

233. $C_4H_3FN_2O_2$

5 Fluorouracil
5-Fluorouracil
Fluorouracil
5-Fluoro-2,4(1H,3H)-pyrimidinedione
Fluroblastin
Fluororuracil
RN: 51-21-8 **MP** (°C)**:** 281
MW: 130.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-02	1.249E+01	21	B416	2 2 1 2 1	
8.533E-02	1.110E+01	22	B321	0 0 0 0 0	pH 4.0
8.533E-02	1.110E+01	22	B332	1 1 0 0 1	pH 4.0
8.533E-02	1.110E+01	22	B388	0 0 0 0 0	
9.379E-02	1.220E+01	22	M317	1 1 1 1 1	
9.379E-02	1.220E+01	25	R023	0 0 0 0 0	
1.356E-01	1.763E+01	25	S471	0 0 0 0 0	
1.382E-01	1.798E+01	25	S471	0 0 0 0 0	
6.940E-02	9.027E+00	25	Z408	0 0 0 0 0	
8.533E-02	1.110E+01	37	B332	0 0 0 0 0	pH 4.0
9.566E-02	1.244E+01	ns	S469	0 0 0 0 0	

234. $C_4H_3IN_2O_2$

5-Iodouracil
5-Iodo-2,4(1H,3H)-pyrimidinedione
5-Iodo-2,4-dihydroxypyrimidine

RN: 696-07-1 **MP** (°C)**:** 274–276 (°dec)
MW: 237.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-02	4.907E+00	25	S471	0 0 0 0 0	
2.072E-02	4.931E+00	25	S471	0 0 0 0 0	
1.060E-02	2.523E+00	25	Z408	0 0 0 0 0	

235. $C_4H_3N_2S$

2-Methyl-1,3,4-thiadiazole
Thiodiazolique methyle

RN: 26584-42-9 **MP** (°C)**:**
MW: 111.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.918E-03	8.800E-01	37	D084	1 0 1 0 1	

236. $C_4H_3N_3O_4$

5-Nitrouracil

RN: 611-08-5 **MP** (°C)**:**
MW: 157.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	3.613E+00	25	Z408	0 0 0 0 0	

237. $C_4H_3N_3O_5$

5-Nitrobarbituric acid
Dilitursaeure

RN: 28176-10-5 **MP** (°C)**:** 176
MW: 173.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	9.000E-01	25.60	F300	1 0 0 0 0	

238. $C_4H_4Br_2O_4$

meso-2,3-Dibromosuccinic acid
meso-Dibrom-bernsteinsaeure
DL-2,3-Dibromosuccinic acid
DL-Dibrom-bernsteinsaeure

RN: 526-78-3 **MP** (°C)**:** 171
MW: 275.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.249E-02	2.000E+01	17	F300	1 0 0 0 2	

239. $C_4H_4Cl_2N_2O_2$

1,3-Dichloro-5-methylhydantoin
2,4-Imidazolidinedione, 1,3-dichloro-5-methyl-
Hydantoin, 1,3-dichloro-5-methyl-

RN: 15216-12-3 **MP** (°C)**:**
MW: 182.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.634E-02	2.991E+00	20	B080	1 0 1 1 0	
4.498E-02	8.232E+00	40	B080	1 0 1 1 1	

240. $C_4H_4Cl_2O_4$

L-2,3-Dichlorosuccinic acid
L(–)-Dichlor-bernsteinsaeure
D-2,3-Dichlorosuccinic acid
D(+)-Dichlor-bernsteinsaeure
2,3-Dichlorosuccinic acid
meso-2,3-Dichlorosuccinic acid

RN: 19922-87-3 **MP** (°C)**:** 168
MW: 186.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.674E+00	5.000E+02	25	H090	0 1 1 1 1	
1.701E-02	3.180E+00	ns	H090	0 2 2 1 2	

241. $C_4H_4N_2$

Succinonitrile
Bersteinsaeure-dinitril

RN: 110-61-2 **MP** (°C)**:** 57
MW: 80.09 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E+00	1.269E+02	20	F300	1 0 0 0 2	

242. $C_4H_4N_2O$
4(3H)-Pyrimidone
4-Hydroxypyrimidine
RN: 51953-17-4 **MP** (°C)**:** 164
MW: 96.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E+00	2.703E+02	20	B050	1 0 0 0 0	

243. $C_4H_4N_2O$
2-Hydroxypyrimidine
2-Pyrimidinol
RN: 51953-13-0 **MP** (°C)**:**
MW: 96.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.252E+00	3.125E+02	20	B050	1 0 0 0 0	

244. $C_4H_4N_2OS$
2-Thiouracil
Thiouracil
4(1H)-Pyrimidinone
RN: 141-90-2 **MP** (°C)**:** 340
MW: 128.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-03	5.996E-01	20	D041	1 0 0 0 0	
5.530E-03	7.087E-01	25	G016	1 2 1 2 2	intrinsic
3.900E-03	4.998E-01	ns	I310	0 0 0 0 0	

245. $C_4H_4N_2O_2$
Uracil
2,4-Dihydroxypyrimidine
RN: 66-22-8 **MP** (°C)**:** 335
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	
2.500E-02	2.802E+00	20	N019	0 0 0 0 0	
3.200E-02	3.587E+00	25	D041	1 0 0 0 1	
3.212E-02	3.600E+00	25	F300	1 0 0 0 1	
2.380E-02	2.668E+00	25	H061	0 0 0 0 0	
4.109E-02	4.605E+00	25	S471	0 0 0 0 0	
4.125E-02	4.624E+00	25	S471	0 0 0 0 0	

(*continued*)

245. $C_4H_4N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-02	3.038E+00	25	Z408	0 0 0 0 0	
4.015E-02	4.500E+00	37	B390	0 0 0 0 0	
2.676E-02	3.000E+00	ns	B177	0 0 0 0 0	

246. $C_4H_4N_2O_2$

4,6-Dihydroxypyrimidine
4,6-Pyrimidinediol
RN: 1193-24-4 **MP** (°C)**:** >300
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.225E-02	2.494E+00	20	B050	1 0 0 0 0	

247. $C_4H_4N_2O_2$

2,4-Dihydroxypyrimidine
RN: 51953-14-1 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	

248. $C_4H_4N_2O_2$

Maleic hydrazide
Dihydropyridazine-3,6-dione
RN: 123-33-1 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.554E-02	3.984E+00	20	B185	0 0 0 0 0	
5.321E-02	5.964E+00	25	B185	0 0 0 0 0	
5.353E-02	6.000E+00	25	B200	1 0 0 0 2	
5.321E-02	5.964E+00	25	M061	1 0 0 0 0	
5.353E-02	6.000E+00	25	M161	1 0 0 0 0	
5.321E-02	5.964E+00	ns	B100	0 0 0 0 0	
6.310E-03	7.072E-01	ns	M163	0 0 0 0 0	EFG
3.554E-02	3.984E+00	ns	N013	0 0 0 0 0	

249. $C_4H_4N_2O_3$
Barbituric acid
Barbitursaeure
RN: 67-52-7 **MP** (°C)**:** 248
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-07	1.900E-05	37	B166	1 0 1 1 1	
5.129E-02	6.569E+00	ns	R424	0 0 0 0 0	
5.129E-02	6.569E+00	ns	R427	0 0 0 0 0	

250. $C_4H_4N_2O_3$
2,4,6-Trihydroxypyrimidine
2,4,6-Pyrimidinetriol
RN: 223674-01-9 **MP** (°C)**:**
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.170E-02	6.623E+00	20	B050	1 0 0 0 0	

251. $C_4H_4O_4$
trans-Fumaric acid
Fumaric acid
Fumarsaeure
RN: 110-17-8 **MP** (°C)**:** 287
MW: 116.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-02	2.295E+00	0	M043	1 0 0 0 1	
3.005E-02	3.488E+00	10	M043	1 0 0 0 1	
4.286E-02	4.975E+00	20	M043	1 0 0 0 1	
5.989E-02	6.951E+00	25	D041	1 0 0 0 1	
6.031E-02	7.000E+00	25	F300	1 0 0 0 0	
5.989E-02	6.951E+00	25	W011	1 2 2 1 1	
6.159E-02	7.149E+00	30	M043	1 0 0 0 1	
9.218E-02	1.070E+01	40	F300	1 0 0 0 2	
9.374E-02	1.088E+01	40	M043	1 0 0 0 1	
9.121E-02	1.059E+01	40	W011	1 2 2 1 2	
1.937E-01	2.248E+01	60	M043	1 0 0 0 1	
2.019E-01	2.344E+01	60	W011	1 2 2 1 1	
4.258E-01	4.943E+01	80	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	D041	1 0 0 0 1	
8.012E-01	9.300E+01	100	F300	1 0 0 0 1	
7.689E-01	8.925E+01	100	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	W011	1 2 2 1 1	
5.248E-02	6.092E+00	ns	R424	0 0 0 0 0	

252. $C_4H_4O_4$

Maleic acid
Maleinsaeure

RN: 110-16-7 **MP** (°C)**:** 138
MW: 116.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.431E+00	2.821E+02	0	M043	1 0 0 0 2	
2.607E+00	3.026E+02	4.99	A339	0 0 0 0 0	
2.872E+00	3.334E+02	10	F300	1 0 0 0 2	
2.872E+00	3.333E+02	10	M043	1 0 0 0 1	
2.880E+00	3.343E+02	9.99	A339	0 0 0 0 0	
3.094E+00	3.591E+02	14.99	A339	0 0 0 0 0	
3.312E+00	3.845E+02	19.99	A339	0 0 0 0 0	
3.547E+00	4.118E+02	20	M043	1 0 0 0 1	
6.789E+00	7.880E+02	22.5	G301	0 0 0 0 0	
3.592E+00	4.170E+02	24.99	A339	0 0 0 0 0	
3.797E+00	4.407E+02	25	D041	1 0 0 0 2	
3.797E+00	4.407E+02	25	F300	1 0 0 0 2	
3.840E+00	4.457E+02	25	H430	0 0 0 0 0	
3.797E+00	4.407E+02	25	W011	1 2 2 1 2	
3.823E+00	4.437E+02	29.99	A339	0 0 0 0 0	
4.081E+00	4.737E+02	30	M043	1 0 0 0 1	
4.117E+00	4.778E+02	34.99	A339	0 0 0 0 0	
4.300E+00	4.991E+02	39.99	A339	0 0 0 0 0	
4.608E+00	5.349E+02	40	M043	1 0 0 0 2	
4.561E+00	5.294E+02	40	W011	1 2 2 1 2	
4.562E+00	5.295E+02	44.99	A339	0 0 0 0 0	
4.677E+00	5.429E+02	49.99	A339	0 0 0 0 0	
4.842E+00	5.620E+02	54.99	A339	0 0 0 0 0	
5.031E+00	5.840E+02	59.99	A339	0 0 0 0 0	
5.516E+00	6.403E+02	60	M043	1 0 0 0 2	
5.151E+00	5.979E+02	60	W011	1 2 2 1 2	
5.166E+00	5.997E+02	64.99	A339	0 0 0 0 0	
6.366E+00	7.389E+02	80	M043	1 0 0 0 2	
6.864E+00	7.967E+02	97.5	D041	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	F300	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	W011	1 2 2 1 2	

253. C_4H_4S

Thiophene
Thiofuran
Thiacyclopentadiene

RN: 110-02-1 **MP** (°C)**:** –38.3
MW: 84.14 **BP** (°C)**:** 84.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-02	3.015E+00	25	K119	1 0 0 0 2	
3.583E-02	3.015E+00	25	P051	2 1 1 2 2	
3.583E-02	3.015E+00	25.00	P007	2 1 2 2 2	

254. $C_4H_5BrO_4$
Bromosuccinic acid
DL-Brombernsteinsaeure
RN: 923-06-8 **MP** (°C)**:**
MW: 196.99 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.092E-01	1.200E+02	15.5	F300	1 0 0 0 1	

255. $C_4H_5ClO_2$
2-Chloroisocrotonic acid
α-Chlor-isocrotonsaeure
RN: 24253-33-6 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.102E-01	6.150E+01	19	F300	1 0 0 0 2	

256. $C_4H_5ClO_2$
2-Chlorocrotonic acid
α-Chlor-crotonsaeure
RN: 600-13-5 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-01	2.100E+01	19	F300	1 0 0 0 1	

257. $C_4H_5ClO_2$
3-Chlorocrotonic acid
β-Chlor-crotonsaeure
RN: 6214-28-4 **MP** (°C)**:** 94
MW: 120.54 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-01	2.220E+01	12.5	F300	1 0 0 0 2	
2.481E-01	2.990E+01	19	F300	1 0 0 0 2	

258. $C_4H_5ClO_2$
3-Chloroisocrotonic acid
β-Chlor-isocrotonsaeure
RN: 6625-00-9 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.037E-01	1.250E+01	7	F300	1 0 0 0 2	
1.560E-01	1.880E+01	19	F300	1 0 0 0 2	

259. $C_4H_5ClO_4$
L-Chlorosuccinic acid
L(–)-Chlor-bernsteinsaeure
D-Chlorosuccinic acid
D(+)-Chlor-bernsteinsaeure
RN: 16045-92-4 **MP** (°C)**:**
MW: 152.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E+00	1.800E+02	20	F300	1 0 0 0 1	
1.193E+00	1.820E+02	20	F300	1 0 0 0 2	

260. $C_4H_5F_3O$
Fluroxene
2,2,2-(Trifluoroethoxy)ethene
Redeptin
Fluoromar
RN: 406-90-6 **MP** (°C)**:**
MW: 126.08 **BP** (°C)**:** 42.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.173E-05	4.000E-03	ns	R028	0 0 0 0 0	

261. C_4H_5N
Pyrrole
Azole
Imidole
RN: 109-97-7 **MP** (°C)**:** –23
MW: 67.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.098E-01	4.762E+01	rt	B099	0 2 0 0 0	

262. C_4H_5N

Methacrylonitrile
2-Methyl-2-propenenitrile

RN: 126-98-7 **MP** (°C)**:** –35.8
MW: 67.09 **BP** (°C)**:** 90.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.692E-01	2.477E+01	25	L096	1 2 0 2 2	

263. $C_4H_5NO_2$

Hymexazol
3-Hydroxy-5-methyl isoxazole
5-Methyl-3(2H)-isoxazolone
Tachigaren
Isoxazolol, 5-methyl-

RN: 10004-44-1 **MP** (°C)**:** 86
MW: 99.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-01	8.500E+01	25	M161	1 0 0 0 2	
8.578E-01	8.500E+01	25	N306	1 0 0 0 1	

264. $C_4H_5NO_2$

Succinimide
2,5-Pyrrolidinedione
Butanimide

RN: 123-56-8 **MP** (°C)**:** 126
MW: 99.09 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.174E-01	9.091E+01	0	M043	1 0 0 0 1	
1.392E+00	1.379E+02	10	M043	1 0 0 0 1	
2.082E+00	2.063E+02	20	M043	1 0 0 0 1	
1.978E+00	1.960E+02	21	F300	1 0 0 0 2	
3.273E+00	3.243E+02	30	M043	1 0 0 0 1	
4.577E+00	4.536E+02	40	M043	1 0 0 0 1	
5.887E+00	5.833E+02	60	M043	1 0 0 0 2	
6.868E+00	6.805E+02	80	M043	1 0 0 0 2	
1.413E+00	1.400E+02	ns	D072	0 0 0 0 1	
1.995E+00	1.977E+02	ns	R424	0 0 0 0 0	

265. C_4H_5NS

Allyl isothiocyanate
Allyl mustardiol
Allylsenfoel

RN: 57-06-7 **MP** (°C)**:** –8
MW: 99.16 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.017E-02	2.000E+00	20	F300	1 0 0 0 0	

266. $C_4H_5N_3O$

Cytosine
2-Oxy-4-amino pyrimidine
2(1H)-Pyrimidinone, 4-amino-

RN: 71-30-7 **MP** (°C)**:** 320
MW: 111.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.555E+00	20	C017	2 0 0 1 0	EFG
6.877E-02	7.641E+00	25	D041	1 0 0 0 1	
7.200E-02	8.000E+00	25	F300	1 0 0 0 0	
6.580E-02	7.311E+00	25	H061	0 0 0 0 0	
6.500E-02	7.222E+00	25	R030	0 0 0 0 0	

267. $C_4H_5N_3OS$

6-Amino-2-thiouracil
2-Mercapto-4-amino-6-hydroxypyrimidine
2-Thio-4-amino-6-hydroxypyrimidine
2-Mercapto-6-aminouracil

RN: 1004-40-6 **MP** (°C)**:**
MW: 143.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	2.563E-01	25	G016	1 2 1 2 2	intrinsic

268. $C_4H_5N_3O_2$

5-Aminouracil
5-Amino-uracil

RN: 932-52-5 **MP** (°C)**:** >300
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.934E-03	5.000E-01	20	F300	1 0 0 0 0	
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	
1.259E-01	1.600E+01	100	F300	1 0 0 0 1	

269. $C_4H_5N_3O_2$
6-Aminouracil
2,4(1H,3H)-Pyrimidinedione, 6-amino
4-Amino-2,6-dihydroxypyrimidine
6-Amino-2,4-pyrimidinediol
4-Amino uracil
RN: 873-83-6 **MP** (°C)**:**
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	

270. $C_4H_5N_3O_2$
2-Methyl-4(5)-nitroimidazole
2-Methyl-5-nitroimidazole
Menidazole
RP 8532
L 581490
RN: 696-23-1 **MP** (°C)**:** 257–258
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E-02	3.010E+00	20	D344	0 0 0 0 0	
2.367E-02	3.009E+00	20	D344	0 0 0 0 0	
2.353E-02	2.991E+00	20	D344	0 0 0 0 0	
2.370E-02	3.012E+00	20	D344	0 0 0 0 0	

271. C_4H_6
1,3-Butadiene
Pyrrolylene
RN: 106-99-0 **MP** (°C)**:** –108.9
MW: 54.09 **BP** (°C)**:** –4.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.359E-02	7.350E-01	25	M001	2 1 2 2 2	

272. C_4H_6
1-Butyne
Ethylacetylene
Ethylethyne
RN: 107-00-6 **MP** (°C)**:** –125.7
MW: 54.09 **BP** (°C)**:** 8.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.306E-02	2.870E+00	25	M001	2 1 2 2 2	

273. $C_4H_6BrNO_4$

5-Bromo-5-nitro-1,3-dioxane
Bronidox
Microcide I
Bronidox L
1,3-Dioxane, 5-bromo-5-nitro-
RN: 30007-47-7 **MP** (°C)**:** 49–50
MW: 212.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.706E-02	5.737E+00	25	L013	1 0 2 1 2	

274. $C_4H_6Cl_2O_2S$

3,4-Dichlorotetrahydrothiophene dioxide
3,4-Dichlorotetrahydrothiophene 1,1-dioxide
3,4-Dichlorosulfolane
DAC PRD
3,4-Dichlorothiolane 1,1-dioxide
RN: 3001-57-8 **MP** (°C)**:** 130
MW: 189.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-02	2.195E+00	20	M061	1 0 0 0 1	

275. $C_4H_6N_2O_2$

2,5-Piperazinedione
Diketopiperazine
RN: 106-57-0 **MP** (°C)**:**
MW: 114.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	1.406E+01	20	B032	1 2 2 1 2	
1.253E-01	1.430E+01	20	M075	2 0 1 1 2	
1.475E-01	1.683E+01	25	B032	1 2 2 1 2	
1.754E-01	2.001E+01	29.80	B032	1 2 2 1 2	

276. $C_4H_6N_2S_4Zn$

Zineb
Zinc ethylenebis(dithiocarbamate)
RN: 12122-67-7 **MP** (°C)**:**
MW: 275.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-06	1.000E-03	20	M061	1 0 0 0 0	
3.627E-05	1.000E-02	rt	M161	0 0 0 0 1	

277. $C_4H_6N_4O_3$
Allantoin
Allantoine
RN: 97-59-6 **MP** (°C)**:** 238
MW: 158.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.303E-02	5.223E+00	20	D041	1 0 0 0 2	
4.755E-02	7.519E+00	c	D004	0 0 0 0 0	
2.040E-01	3.226E+01	h	D004	0 0 0 0 0	
2.530E-02	4.000E+00	ns	D072	0 0 0 0 1	

278. $C_4H_6N_4O_3S_2$
Acetazolamide
5-Acetamido-1,3,4-thiadiazole-2-sulfonamide
RN: 59-66-5 **MP** (°C)**:** 258
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.001E-01	15	K024	1 2 1 1 2	
2.249E-03	4.998E-01	20	D041	1 0 0 0 0	
3.200E-03	7.112E-01	25	C415	1 0 0 1 0	
2.216E-03	4.925E-01	25	F415	0 0 0 0 0	Average
4.409E-03	9.799E-01	30	E049	2 0 2 2 2	
5.174E-03	1.150E+00	37	C054	2 0 2 1 2	
2.880E-03	6.400E-01	amb	L434	0 0 0 0 0	
>2.25E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.144E-03	9.210E-01	ns	I304	0 0 0 0 0	
4.500E-04	1.000E-01	ns	K444	0 0 0 0 0	
4.365E-03	9.701E-01	ns	R428	0 0 0 0 0	

279. C_4H_6O
Vinyl ether
1,1′-Oxybisethene
Divinyl ether
RN: 109-93-3 **MP** (°C)**:**
MW: 70.09 **BP** (°C)**:** 28.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.490E-02	5.250E+00	37	R047	0 0 0 0 0	
5.487E-01	3.846E+01	ns	R028	0 0 0 0 0	

280. C_4H_6O
Crotonaldehyde
But-*trans*-enal
RN: 4170-30-3 **MP** (°C)**:** –76.5
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+2.14E+00	+1.50E+02	ns	S460	0 0 0 0 0	

281. C_4H_6O
α-Methylacrolein
α-Methyl-acrolein
RN: 78-85-3 **MP** (°C)**:**
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.089E-01	5.670E+01	20	F300	1 0 0 0 2	
1.236E+00	8.663E+01	ns	S460	0 0 0 0 0	

282. C_4H_6O
trans-Crotonaldehyde
Crotonaldehyd
RN: 123-73-9 **MP** (°C)**:** –77
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.140E+00	1.500E+02	20	F300	1 0 0 0 1	

283. $C_4H_6O_2$
Diacetyl
2,3-Butanedione
RN: 431-03-8 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E+00	2.000E+02	15	F300	1 0 0 0 1	
2.323E+00	2.000E+02	20	D041	1 0 0 0 1	

284. $C_4H_6O_2$
Methyl acrylate
Acrylic acid methyl ester
2-Propenoic acid methyl ester
RN: 96-33-3 **MP** (°C)**:** –76.5
MW: 86.09 **BP** (°C)**:** 70

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.742E-01	4.943E+01	30	L096	1 2 0 2 1	

285. $C_4H_6O_2$
trans-Crotonic acid
trans-Crotonsaeure
RN: 3724-65-0 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.989E-01	8.600E+01	25	F300	1 0 0 0 1	
4.600E+00	3.960E+02	40	F300	1 0 0 0 2	

286. $C_4H_6O_2$
Vinyl acetate
Vinylacetate
RN: 108-05-4 **MP** (°C)**:** –100
MW: 86.09 **BP** (°C)**:** 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.136E-01	2.700E+01	50	L097	1 1 1 1 1	

287. $C_4H_6O_2$
Crotonic acid
2-Butenoic acid
3-Methylacrylic acid
RN: 107-93-7 **MP** (°C)**:** 73
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.882E-01	7.647E+01	20	D041	1 0 0 0 2	

288. $C_4H_6O_2$
α-Butyrolacetone
3-Hydroxybutanoic acid β-lactone
RN: 3068-88-0 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E+00	1.327E+02	18	I313	0 0 0 0 0	

289. $C_4H_6O_2S_4$

bis(Methylxanthogen) disulfide
Dimethylxanthogen disulfide
Methyl dixanthogen

RN: 1468-37-7 **MP** (°C)**:** 22.75
MW: 214.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.465E-02	25	H102	1 2 1 2 2	

290. $C_4H_6O_3$

Acetic anhydride
Essigsaeure-anhydrid

RN: 108-24-7 **MP** (°C)**:** –73
MW: 102.09 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E+00	1.200E+02	20	F300	1 0 0 0 2	

291. $C_4H_6O_4$

Methylmalonic acid
Acide methylmalonique
Methyl-malonsaeure

RN: 516-05-2 **MP** (°C)**:** 129.5
MW: 118.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	3.070E+02	0	F300	1 0 0 0 2	
3.743E+00	4.420E+02	0	M051	1 0 0 0 2	
4.954E+00	5.850E+02	15	M051	1 0 0 0 2	
5.750E+00	6.790E+02	25	M051	1 0 0 0 2	
4.071E+00	4.808E+02	50	F300	1 0 0 0 2	
7.748E+00	9.150E+02	50	M051	1 0 0 0 2	

292. $C_4H_6O_4$

Succinic acid
Bernsteinsaeure

RN: 110-15-6 **MP** (°C)**:** 185
MW: 118.09 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.363E-01	2.790E+01	0	L041	1 0 0 1 2	
2.273E-01	2.684E+01	0	M020	1 0 0 1 1	
2.306E-01	2.724E+01	0	M043	1 0 0 0 1	

(*continued*)

292. $C_4H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.892E-01	3.415E+01	4.99	A339	0 0 0 0 0	
3.569E-01	4.215E+01	10	M043	1 0 0 0 1	
3.616E-01	4.271E+01	9.99	A339	0 0 0 0 0	
3.854E-01	4.551E+01	11.85	L064	2 2 2 1 2	
4.518E-01	5.335E+01	14.99	A339	0 0 0 0 0	
4.102E-01	4.843E+01	15	F055	1 2 2 2 2	
4.149E-01	4.900E+01	15	L041	1 0 0 1 1	
4.149E-01	4.900E+01	15	M051	1 0 0 0 1	
4.912E-01	5.800E+01	17.50	F300	1 0 0 0 1	
4.974E-01	5.874E+01	18	L064	2 2 2 1 2	
5.661E-01	6.685E+01	19.99	A339	0 0 0 0 0	
5.392E-01	6.367E+01	20	D041	1 0 0 0 1	
5.019E-01	5.927E+01	20	F055	1 2 2 2 2	
5.420E-01	6.400E+01	20	F300	1 0 0 0 2	
4.912E-01	5.800E+01	20	L041	1 0 0 1 1	
5.466E-01	6.455E+01	20	M043	1 0 0 0 1	
5.510E-01	6.507E+01	20	M153	1 0 0 0 0	cal. from fitted equation
4.632E-01	5.470E+01	20	M171	1 0 0 0 1	
5.716E-01	6.750E+01	20	W026	1 0 1 1 1	average of 2
6.344E-01	7.492E+01	23.75	L064	2 2 2 1 2	
6.829E-01	8.064E+01	24.99	A339	0 0 0 0 0	
5.930E-01	7.003E+01	25	D061	1 0 0 0 2	
6.032E-01	7.124E+01	25	F055	1 2 2 2 2	
6.849E-01	8.088E+01	25	H430	0 0 0 0 0	
6.518E-01	7.697E+01	25	M020	1 0 0 1 2	
6.634E-01	7.834E+01	25	M153	1 0 0 0 0	cal. from fitted equation
7.402E-01	8.741E+01	28	D050	1 2 1 2 2	
8.003E-01	9.451E+01	29.99	A339	0 0 0 0 0	
8.047E-01	9.502E+01	30	M043	1 0 0 0 2	
8.047E-01	9.502E+01	30	M153	1 0 0 0 0	cal. from fitted equation
8.849E-01	1.045E+02	30	W026	1 0 1 1 2	average of 2
9.508E-01	1.123E+02	34.99	A339	0 0 0 0 0	
8.976E-01	1.060E+02	35	L041	1 0 0 1 2	
9.742E-01	1.150E+02	35	M153	1 0 0 0 0	cal. from fitted equation
1.145E+00	1.353E+02	39.99	A339	0 0 0 0 0	
1.149E+00	1.357E+02	40	B088	1 0 0 0 2	
1.181E+00	1.394E+02	40	M043	1 0 0 0 2	
1.168E+00	1.379E+02	40	M153	1 0 0 0 0	cal. from fitted equation
1.377E+00	1.627E+02	44.99	A339	0 0 0 0 0	
1.600E+00	1.889E+02	49.99	A339	0 0 0 0 0	
1.524E+00	1.800E+02	50	L041	1 0 0 1 2	
1.633E+00	1.929E+02	50	M020	1 0 0 1 2	
1.842E+00	2.175E+02	54.99	A339	0 0 0 0 0	
2.048E+00	2.418E+02	59.99	A339	0 0 0 0 0	
2.232E+00	2.636E+02	60	M043	1 0 0 0 2	
2.398E+00	2.832E+02	64.99	A339	0 0 0 0 0	
2.380E+00	2.810E+02	65	L041	1 0 0 1 2	
3.238E+00	3.824E+02	75	F300	1 0 0 0 2	
3.191E+00	3.768E+02	75	M020	1 0 0 1 2	

(*continued*)

292. $C_4H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E+00	4.145E+02	80	M043	1 0 0 0 2	
8.515E-01	1.006E+02	84.30	B118	1 0 0 0 2	unit assumed
4.636E+00	5.475E+02	100	D041	1 0 0 0 2	
4.738E+00	5.595E+02	100	M043	1 0 0 0 2	
6.821E-01	8.054E+01	rt	H431	0 0 0 0 0	

293. $C_4H_6O_4$

Methyl oxalate
Oxalic acid ethyl ester
Oxalsaeure-monoaethyl ester

RN: 553-90-2 **MP** (°C)**:** 54.0
MW: 118.09 **BP** (°C)**:** 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-01	3.549E+01	.1	K079	1 0 0 0 2	
6.900E-01	8.148E+01	11.1	K079	1 0 0 0 2	
1.029E+00	1.216E+02	19.5	K079	1 0 0 0 2	
5.106E-01	6.030E+01	25	F300	1 0 0 0 2	
1.489E+00	1.758E+02	27.1	K079	1 0 0 0 2	
1.867E+00	2.204E+02	31.9	K079	1 0 0 0 2	
2.978E+00	3.516E+02	44.4	K079	1 0 0 0 2	
3.372E+00	3.982E+02	49.2	K079	1 0 0 0 2	
3.589E+00	4.238E+02	51.0	K079	1 0 0 0 2	
3.839E+00	4.533E+02	53.0	K079	1 0 0 0 2	
4.783E+00	5.649E+02	75.0	K079	1 0 0 0 2	
4.939E+00	5.832E+02	79.3	K079	1 0 0 0 2	
5.678E+00	6.705E+02	96.1	K079	1 0 0 0 2	
4.929E-01	5.820E+01	rt	D021	0 0 1 1 2	

294. $C_4H_6O_5$

D-Malic acid
D(–)-Aepfelsaeure

RN: 636-61-3 **MP** (°C)**:** 100
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.397E+00	4.555E+02	4.99	A339	0 0 0 0 0	
3.542E+00	4.749E+02	9.99	A339	0 0 0 0 0	
3.695E+00	4.954E+02	14.99	A339	0 0 0 0 0	
3.878E+00	5.200E+02	19.99	A339	0 0 0 0 0	
4.030E+00	5.403E+02	24.99	A339	0 0 0 0 0	
4.146E+00	5.560E+02	29.99	A339	0 0 0 0 0	
4.282E+00	5.742E+02	34.99	A339	0 0 0 0 0	
4.441E+00	5.955E+02	39.99	A339	0 0 0 0 0	
4.544E+00	6.094E+02	44.99	A339	0 0 0 0 0	

(*continued*)

294. $C_4H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E+00	6.328E+02	49.99	A339	0 0 0 0 0	
4.840E+00	6.490E+02	54.99	A339	0 0 0 0 0	
4.976E+00	6.672E+02	59.99	A339	0 0 0 0 0	
5.119E+00	6.865E+02	64.99	A339	0 0 0 0 0	

295. $C_4H_6O_5$

Diglycolic acid
Di-glykolsaeure

RN: 110-99-6 **MP** (°C)**:** 148
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E+00	2.140E+02	5.09	A340	0 0 0 0 0	
1.932E+00	2.590E+02	10.99	A340	0 0 0 0 0	
2.522E+00	3.382E+02	15.59	A340	0 0 0 0 0	
2.668E+00	3.577E+02	20.59	A340	0 0 0 0 0	
2.834E+00	3.801E+02	23.49	A340	0 0 0 0 0	
3.252E+00	4.361E+02	28.09	A340	0 0 0 0 0	
3.645E+00	4.887E+02	37.49	A340	0 0 0 0 0	
3.794E+00	5.087E+02	39.99	A340	0 0 0 0 0	
4.061E+00	5.445E+02	47.99	A340	0 0 0 0 0	
4.135E+00	5.545E+02	49.99	A340	0 0 0 0 0	
4.353E+00	5.837E+02	54.49	A340	0 0 0 0 0	
4.508E+00	6.044E+02	59.49	A340	0 0 0 0 0	
4.631E+00	6.209E+02	64.99	A340	0 0 0 0 0	
4.776E+00	6.404E+02	69.99	A340	0 0 0 0 0	
4.877E+00	6.540E+02	74.99	A340	0 0 0 0 0	
4.969E+00	6.663E+02	79.89	A340	0 0 0 0 0	
5.067E+00	6.794E+02	83.99	A340	0 0 0 0 0	
5.125E+00	6.872E+02	88.19	A340	0 0 0 0 0	

296. $C_4H_6O_5$

DL-Malic acid
Malic acid

RN: 6915-15-7 **MP** (°C)**:** 131.5
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.512E+00	4.709E+02	0	M043	1 0 0 0 1	
3.820E+00	5.122E+02	10	M043	1 0 0 0 2	
4.158E+00	5.575E+02	20	M043	1 0 0 0 2	
4.414E+00	5.918E+02	25	H430	0 0 0 0 0	
4.401E+00	5.902E+02	26	D041	1 0 0 0 2	
4.415E+00	5.920E+02	26	F300	1 0 0 0 2	

(*continued*)

296. $C_4H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.605E+00	7.516E+02	30	D062	1 0 1 1 0	data given in normality
4.475E+00	6.000E+02	30	M043	1 0 0 0 2	
4.794E+00	6.429E+02	40	M043	1 0 0 0 2	
5.442E+00	7.297E+02	60	M043	1 0 0 0 2	
5.998E+00	8.043E+02	79	D041	1 0 0 0 2	
6.033E+00	8.089E+02	79	F300	1 0 0 0 2	
6.126E+00	8.214E+02	80	M043	1 0 0 0 2	

297. $C_4H_6O_6$

meso-Tartaric acid
meso-Weinsaeure

RN: 147-73-9 **MP** (°C)**:** 147
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	3.360E+02	0	F300	1 0 0 0 2	
3.702E+00	5.556E+02	15	D041	1 0 0 0 2	
3.731E+00	5.600E+02	15	F300	1 0 0 0 1	
3.731E+00	5.600E+02	20	F300	1 0 0 0 1	

298. $C_4H_6O_6$

D-(–)-Tartaric acid
D-(–)-Dihydroxysuccinic acid

RN: 147-71-7 **MP** (°C)**:** 173
MW: 150.09 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.564E+00	5.349E+02	0	M043	1 0 0 0 2	
3.348E+00	5.024E+02	4.99	A339	0 0 0 0 0	
2.350E+00	3.528E+02	10	D020	1 2 1 1 2	
3.715E+00	5.575E+02	10	M043	1 0 0 0 2	
3.431E+00	5.149E+02	9.99	A339	0 0 0 0 0	
3.499E+00	5.251E+02	14.99	A339	0 0 0 0 0	
3.553E+00	5.332E+02	19.99	A339	0 0 0 0 0	
3.875E+00	5.816E+02	20	M043	1 0 0 0 2	
3.629E+00	5.447E+02	24.99	A339	0 0 0 0 0	
2.459E+00	3.691E+02	25	D020	1 2 1 1 2	
3.973E+00	5.963E+02	25	F017	1 0 0 0 2	
3.706E+00	5.562E+02	29.99	A339	0 0 0 0 0	
4.060E+00	6.094E+02	30	M043	1 0 0 0 2	
3.791E+00	5.690E+02	34.99	A339	0 0 0 0 0	
3.846E+00	5.773E+02	39.99	A339	0 0 0 0 0	
4.249E+00	6.377E+02	40	M043	1 0 0 0 2	
3.926E+00	5.892E+02	44.99	A339	0 0 0 0 0	

(*continued*)

298. $C_4H_6O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E+00	6.036E+02	49.99	A339	0 0 0 0 0	
4.104E+00	6.160E+02	54.99	A339	0 0 0 0 0	
4.157E+00	6.238E+02	59.99	A339	0 0 0 0 0	
4.581E+00	6.875E+02	60	M043	1 0 0 0 2	
4.232E+00	6.352E+02	64.99	A339	0 0 0 0 0	
4.876E+00	7.319E+02	80	M043	1 0 0 0 2	
5.159E+00	7.743E+02	100	M043	1 0 0 0 2	

299. $C_4H_6O_6$

L-Tartaric acid
L(+)-Weinsaeure
L(+)-Tartaric acid

RN: 87-69-4 **MP** (°C)**:** 169
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.565E+00	5.350E+02	0	F300	1 0 0 0 2	
3.564E+00	5.349E+02	0	F302	1 0 0 0 2	
3.634E+00	5.455E+02	5	F302	1 0 0 0 2	
3.702E+00	5.556E+02	10	F302	1 0 0 0 2	
3.791E+00	5.690E+02	15	F302	1 0 0 0 2	
3.878E+00	5.820E+02	20	F300	1 0 0 0 2	
3.875E+00	5.816E+02	20	F302	1 0 0 0 2	
3.965E+00	5.951E+02	25	F302	1 0 0 0 2	
4.060E+00	6.094E+02	30	F302	1 0 0 0 2	
4.158E+00	6.241E+02	35	F302	1 0 0 0 2	
4.249E+00	6.377E+02	40	F302	1 0 0 0 2	
4.325E+00	6.491E+02	45	F302	1 0 0 0 2	
4.397E+00	6.600E+02	50	F300	1 0 0 0 1	
4.404E+00	6.610E+02	50	F302	1 0 0 0 2	
4.485E+00	6.732E+02	55	F302	1 0 0 0 2	
4.568E+00	6.855E+02	60	F302	1 0 0 0 2	
4.644E+00	6.970E+02	65	F302	1 0 0 0 2	
4.726E+00	7.093E+02	70	F302	1 0 0 0 2	
4.802E+00	7.207E+02	75	F302	1 0 0 0 2	
4.876E+00	7.319E+02	80	F302	1 0 0 0 2	
4.954E+00	7.436E+02	85	F302	1 0 0 0 2	
5.026E+00	7.543E+02	90	F302	1 0 0 0 2	
5.095E+00	7.647E+02	95	F302	1 0 0 0 2	
5.157E+00	7.740E+02	100	F300	1 0 0 0 2	
5.159E+00	7.743E+02	100	F302	1 0 0 0 2	

300. $C_4H_6O_6$

DL-Tartaric acid
DL-Weinsaeure
Tartaric acid (racemic)

RN: 133-37-9 **MP** (°C)**:** 206
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.279E+00	3.421E+02	0	D039	2 2 1 2 0	EFG
5.630E-01	8.450E+01	0	D041	1 0 0 0 2	
5.084E-01	7.630E+01	0	F300	1 0 0 0 2	
5.049E-01	7.579E+01	0	M043	1 0 0 0 1	
2.333E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
7.298E-01	1.095E+02	10	M043	1 0 0 0 2	
2.350E+00	3.528E+02	20	D039	2 2 1 2 0	EFG
1.138E+00	1.708E+02	20	D041	1 0 0 0 2	
1.139E+00	1.710E+02	20	F300	1 0 0 0 2	
1.016E+00	1.525E+02	20	M043	1 0 0 0 2	
2.459E+00	3.690E+02	25	D039	2 2 1 2 2	EFG
1.179E+00	1.770E+02	25	F017	1 0 0 0 2	
1.026E+01	1.540E+03	25	K040	1 0 2 1 2	
2.483E+00	3.726E+02	30	D039	2 2 1 2 0	EFG
1.341E+00	2.013E+02	30	M043	1 0 0 0 2	
2.563E+00	3.846E+02	40	D039	2 2 1 2 0	EFG
1.799E+00	2.701E+02	40	M043	1 0 0 0 2	
2.612E+00	3.921E+02	50	D039	2 2 1 2 0	EFG
2.687E+00	4.033E+02	60	D039	2 2 1 2 0	EFG
2.612E+00	3.921E+02	60	M043	1 0 0 0 2	
2.750E+00	4.128E+02	70	D039	2 2 1 2 0	EFG
2.811E+00	4.220E+02	80	D039	2 2 1 2 0	EFG
3.299E+00	4.952E+02	80	M043	1 0 0 0 2	
2.860E+00	4.292E+02	90	D039	2 2 1 2 0	EFG
2.920E+00	4.382E+02	100	D039	2 2 1 2 0	EFG
4.324E+00	6.490E+02	100	D041	1 0 0 0 2	
4.331E+00	6.500E+02	100	F300	1 0 0 0 1	
3.863E+00	5.798E+02	100	M043	1 0 0 0 2	

301. C_4H_7Br

4-Bromo-1-butene
1-Bromo-3-butene
Homoallyl bromide
4-Bromobutene-1
3-Butenyl bromide

RN: 5162-44-7 **MP** (°C)**:**
MW: 135.01 **BP** (°C)**:** 98.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.660E-03	7.642E-01	25	M342	1 0 1 1 2	

302. $C_4H_7BrN_2O_2$

Propanamide, *N*-(aminocarbonyl)-2-bromo-
(2-Bromopropionyl)urea
α-Bromopropionylurea

RN: 14299-55-9 **MP** (°C)**:**
MW: 195.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.581E-01	5.033E+01	ns	F056	0 2 2 2 1	

303. $C_4H_7BrO_2$

α-Bromobutyric acid
DL-2-Bromobutyric acid
DL-Brombuttersaeure

RN: 80-58-0 **MP** (°C)**:** –4
MW: 167.01 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.191E-01	7.000E+01	ns	F300	1 0 0 0 0	

304. C_4H_7Cl

1-Chloro-2-butene
1-Chloro-2-methylpropene-2
α-Methylallyl chloride

RN: 591-97-9 **MP** (°C)**:**
MW: 90.55 **BP** (°C)**:** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-02	9.990E-01	ns	M061	0 0 0 0 0	

305. $C_4H_7Cl_2O_4P$

Dichlorvos
O,O-Dimethyl *O*-2-dichlorovinyl phosphate

RN: 62-73-7 **MP** (°C)**:**
MW: 220.98 **BP** (°C)**:** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-02	9.901E+00	ns	M061	0 0 0 0 0	
4.525E-02	1.000E+01	rt	M161	0 0 0 0 1	

306. $C_4H_7Cl_3O$

1,1,1-Trichloro-*tert*-butanol
Acetonchloroform
Chloreton

RN: 57-15-8 **MP** (°C)**:** 98
MW: 177.46 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.508E-02	8.000E+00	20	F300	1 0 0 0 0	
4.467E-02	7.927E+00	ns	R424	0 0 0 0 0	
4.467E-02	7.927E+00	ns	R427	0 0 0 0 0	

307. C_4H_7N

n-Butyroniitrile
γ-Butyronitrile
Propyl cyanide
1-Cyanopropane
n-Butyronitrile

RN: 109-74-0 **MP** (°C)**:** –112
MW: 69.11 **BP** (°C)**:** 115–117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.446E-02	3.764E+00	25	B004	0 0 0 0 0	

308. $C_4H_7NO_2S$

4-Thiazolidinecarboxylic acid
Thiazolidine-4-carboxylic acid
γ-Thiaproline
4-Carboxythiazolidine
Detoxepa
Thiaproline

RN: 444-27-9 **MP** (°C)**:** 196–201
MW: 133.17 **BP** (°C)**:** 350.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.930E+01	21	B414	1 0 0 1 1	

309. $C_4H_7NO_3$

N-Acetyl glycine
Aceturic acid
Glycin-*N*-acetat
Glycine-*N*-acetate

RN: 543-24-8 **MP** (°C)**:** 206
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.246E-01	2.630E+01	15	F300	1 0 0 0 2	

310. $C_4H_7NO_4$

Butanoic acid, 4-amino-2-hydroxy-4-oxo-
D-β-Malaminsaeure
r-β-Malaminsaeure

RN: 82310-91-6 **MP** (°C)**:** 149
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.903E-01	3.865E+01	18	L039	1 0 0 0 2	
5.255E-01	6.994E+01	18	L039	1 0 0 0 2	

311. $C_4H_7NO_4$

DL-Aspartic acid
DL-2-Aminobutanedioic acid

RN: 617-45-8 **MP** (°C)**:**
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.367E-02	3.151E+00	0	D018	2 2 2 1 2	
2.420E-02	3.221E+00	4.99	A405	2 0 1 1 2	
3.140E-02	4.179E+00	9.99	A405	2 0 1 1 2	
3.910E-02	5.204E+00	14.99	A405	2 0 1 1 2	
4.850E-02	6.456E+00	19.99	A405	2 0 1 1 2	
5.900E-02	7.853E+00	24.99	A405	2 0 1 1 2	
6.081E-02	8.094E+00	25	D018	2 2 2 1 2	
6.110E-02	8.133E+00	25	D041	1 0 0 0 1	
7.260E-02	9.663E+00	29.99	A405	2 0 1 1 2	
8.770E-02	1.167E+01	33.99	A405	2 0 1 1 2	
8.950E-02	1.191E+01	34.99	A405	2 0 1 1 2	
1.069E-01	1.423E+01	38.99	A405	2 0 1 1 2	
1.109E-01	1.476E+01	39.99	A405	2 0 1 1 2	
1.293E-01	1.721E+01	44.99	A405	2 0 1 1 2	
1.561E-01	2.078E+01	49.49	A405	2 0 1 1 2	
1.544E-01	2.055E+01	50	D018	2 2 2 1 2	
1.812E-01	2.412E+01	54.99	A405	2 0 1 1 2	
2.170E-01	2.888E+01	58.99	A405	2 0 1 1 2	

(*continued*)

311. $C_4H_7NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.543E-01	3.385E+01	61.99	A405	2 0 1 1 2	
3.101E-01	4.128E+01	65.99	A405	2 0 1 1 2	
3.284E-01	4.371E+01	68.99	A405	2 0 1 1 2	
3.646E-01	4.853E+01	70.99	A405	2 0 1 1 2	
3.437E-01	4.575E+01	75	D018	2 2 2 1 2	
3.434E-01	4.571E+01	75	D041	1 0 0 0 2	

312. $C_4H_7NO_4$

Iminodiacetic acid
Imino-diessigsaeure

RN: 142-73-4 **MP** (°C)**:** 247.5
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.781E-01	2.370E+01	5	F300	1 0 0 0 2	

313. $C_4H_7NO_4$

L-Aspartic acid
Aspartic acid
L(+)-Asparaginsaeure
L-(+)-Asparaginic acid
L-(+)-Aspartic acid

RN: 56-84-8 **MP** (°C)**:** 270.5
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-02	2.230E+00	0	D018	2 2 2 1 2	
1.780E-02	2.369E+00	4.99	A405	2 0 1 1 2	
2.170E-02	2.888E+00	9.99	A405	2 0 1 1 2	
2.570E-02	3.421E+00	14.99	A405	2 0 1 1 2	
3.160E-02	4.206E+00	19.99	A405	2 0 1 1 2	
3.170E-02	4.220E+00	20	B032	1 2 2 1 2	
3.750E-02	4.991E+00	24.99	A405	2 0 1 1 2	
3.770E-02	5.018E+00	25	B032	1 2 2 1 2	
4.030E-02	5.364E+00	25	D018	2 2 2 1 2	
3.738E-02	4.975E+00	25	D041	1 0 0 0 0	
3.805E-02	5.064E+00	25	G315	0 0 0 0 0	
3.719E-02	4.950E+00	25	J303	0 0 0 0 0	
3.644E-02	4.850E+00	27	D036	0 0 0 0 0	
4.469E-02	5.948E+00	29.80	B032	1 2 2 1 2	
4.550E-02	6.056E+00	29.99	A405	2 0 1 1 2	
5.320E-02	7.081E+00	33.99	A405	2 0 1 1 2	
6.520E-02	8.678E+00	39.99	A405	2 0 1 1 2	
6.348E-02	8.450E+00	40	J303	0 0 0 0 0	

(*continued*)

313. $C_4H_7NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.610E-02	1.013E+01	44.99	A405	2 0 1 1 2	
9.304E-02	1.238E+01	50	D018	2 2 2 1 2	
9.110E-02	1.213E+01	50.99	A405	2 0 1 1 2	
1.013E-01	1.348E+01	54.99	A405	2 0 1 1 2	
1.216E-01	1.619E+01	59.99	A405	2 0 1 1 2	
1.232E-01	1.640E+01	60	J303	0 0 0 0 0	
1.316E-01	1.752E+01	62.99	A405	2 0 1 1 2	
1.440E-01	1.917E+01	64.99	A405	2 0 1 1 2	
1.498E-01	1.994E+01	66.99	A405	2 0 1 1 2	
1.725E-01	2.296E+01	69.99	A405	2 0 1 1 2	
1.985E-01	2.642E+01	75	D018	2 2 2 1 2	
2.100E-01	2.795E+01	75	D041	1 0 0 0 2	
2.885E-01	3.840E+01	99	M160	2 1 1 1 0	
3.750E-02	4.991E+00	ns	M025	0 2 0 1 2	
3.738E-02	4.975E+00	rt	H431	0 0 0 0 0	

314. $C_4H_7NO_4$

L-β-Malamidic acid
L-β-Malaminsaeure

RN: 57229-74-0 **MP** (°C)**:** 149
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.242E-01	6.977E+01	18	L039	1 0 0 0 2	

315. $C_4H_7N_2O_4$

Glycine dipeptide

RN: **MP** (°C)**:**
MW: 147.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E+00	2.086E+02	20	B032	1 2 2 1 2	
1.534E+00	2.257E+02	25	B032	1 2 2 1 2	
1.540E+00	2.266E+02	25.1	N024	0 0 0 0 0	
1.546E+00	2.275E+02	25.1	N026	0 0 0 0 0	
1.647E+00	2.423E+02	29.80	B032	1 2 2 1 2	

316. $C_4H_7N_3O$
Creatinine
Kreatinin
RN: 60-27-5 **MP** (°C)**:** 220.5
MW: 113.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.075E-01	8.004E+01	16	D041	1 0 0 0 1	
7.081E-01	8.010E+01	16	F300	1 0 0 0 2	

317. C_4H_8
1-Butene
α-Butene
Ethylethylene
α-Butylene
1-Butylene
Butene-1
RN: 106-98-9 **MP** (°C)**:** –185
MW: 56.11 **BP** (°C)**:** –6.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.957E-03	2.220E-01	25	M001	2 1 2 2 2	
1.210E-02	6.791E-01	38	B123	1 2 1 1 2	
1.582E-02	8.876E-01	71	B123	1 2 1 1 2	
2.746E-02	1.541E+00	104	B123	1 2 1 1 2	
3.526E-02	1.979E+00	138	B123	1 2 1 1 2	
3.858E-02	2.165E+00	144.00	B123	1 2 1 1 2	

318. C_4H_8
Isobutylene
2-Methylpropene
RN: 115-11-7 **MP** (°C)**:** –140.3
MW: 56.11 **BP** (°C)**:** –6.90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-03	2.630E-01	25	M001	2 1 2 2 2	

319. $C_4H_8Cl_2$

2,3-Dichlorobutane
Butane, 2,3-dichloro-
RN: 7581-97-7 **MP** (°C)**:** –80
MW: 127.01 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-02	1.817E+00	0	L103	1 0 0 0 2	unit assumed
4.422E-03	5.617E-01	20	L103	1 0 0 0 2	unit assumed
1.464E-03	1.860E-01	30	L103	1 0 0 0 2	unit assumed
1.755E-03	2.230E-01	40	L103	1 0 0 0 2	unit assumed

320. $C_4H_8Cl_2O$

sym-Dichloroethyl ether
2,2′-Dichlorodiethylether
RN: 111-44-4 **MP** (°C)**:** –50
MW: 143.01 **BP** (°C)**:** 66

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.060E-02	1.010E+01	20	D052	1 1 0 0 0	
7.403E-02	1.059E+01	20	M062	1 0 0 0 2	

321. $C_4H_8Cl_2OS$

β,β′-Dichlorodiethylsulfoxide
β,β′-Dichlor-diaethylsulfoxid
RN: 5819-08-9 **MP** (°C)**:**
MW: 175.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.854E-02	1.200E+01	20	F300	1 0 0 0 1	

322. $C_4H_8Cl_2O_2S$

β,β′-Dichlorodiethylsulfone
β,β′-Dichlor-diaethylsulfon
RN: 471-03-4 **MP** (°C)**:**
MW: 191.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.140E-02	6.000E+00	20	F300	1 0 0 0 0	
1.256E-01	2.400E+01	100	F300	1 0 0 0 1	

323. $C_4H_8Cl_2S$

Mustard gas
Sulfure β′-ethyl dichlore
β,β′-Dichlor-diaethylsulfid
RN: 505-60-2 **MP** (°C)**:**
MW: 159.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.337E-03	6.900E-01	25	F300	1 0 0 0 1	
3.017E-03	4.800E-01	c	B079	0 0 1 1 1	

324. $C_4H_8Cl_3O_4P$

Trichlorfon
O,O-Dimethyl (1-hydroxy-2,2,2-trichloroethyl)phosphonate
RN: 52-68-6 **MP** (°C)**:** 83.5
MW: 257.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.982E-01	1.540E+02	25	M161	1 0 0 0 2	
4.255E-01	1.095E+02	ns	M061	0 0 0 0 2	

325. $C_4H_8N_2O_2$

Dimethylglyoxime
Dimethylglyoxim
RN: 95-45-4 **MP** (°C)**:** 240.5
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.167E-03	6.000E-01	20	F300	1 0 0 0 0	
3.100E-02	3.600E+00	80	F300	1 0 0 0 1	
5.081E-02	5.900E+00	100	F300	1 0 0 0 1	

326. $C_4H_8N_2O_2$

Succinamide
Bersteinsaeure-diamid
RN: 110-14-5 **MP** (°C)**:** 260
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.858E-02	4.480E+00	15	D041	1 0 0 0 1	
2.842E-02	3.300E+00	15	F300	1 0 0 0 1	
8.534E-01	9.910E+01	100	D041	1 0 0 0 2	
3.445E-04	4.000E-02	c	L055	0 0 0 0 2	
9.463E-03	1.099E+00	h	L055	0 0 0 0 1	
2.818E-02	3.273E+00	ns	R424	0 0 0 0 0	

327. $C_4H_8N_2O_3$
β-Alanine hydantoic acid
β-Uramidopropionic acid
Glycine, *N*-(aminocarbonyl)-*N*-methyl-
RN: 30565-25-4 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	2.087E+01	25	M024	1 2 0 1 2	

328. $C_4H_8N_2O_3$
N-Nitroso-*N*-methylurethane
N-Nitroso-*N*-methyl-urethan
RN: 615-53-2 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	3.699E+01	24	M031	1 1 1 1 1	

329. $C_4H_8N_2O_3$
N-Glycylglycine
Diglycine
RN: 556-50-3 **MP** (°C)**:** 215
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E+00	1.656E+02	21	F300	1 0 0 0 2	
1.740E+00	2.299E+02	24.99	B441	0 0 0 0 0	
1.399E+00	1.848E+02	25	G092	2 1 1 1 1	
1.399E+00	1.848E+02	25	G315	0 0 0 0 0	
1.430E+00	1.890E+02	25.1	N027	1 2 2 2 2	
1.512E+00	1.998E+02	ns	M025	0 2 0 1 2	

330. $C_4H_8N_2O_3$
α-Alanine hydantoic acid
Methylhydantoic acid
RN: 77340-50-2 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-01	2.550E+01	25	M024	1 2 0 1 2	
1.930E-01	2.550E+01	ns	M025	0 2 0 1 2	

331. $C_4H_8N_2O_3$

Asparagine
L-Asparagine
L-Asparagin

RN: 70-47-3 **MP** (°C)**:** 235
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.509E-02	8.600E+00	0	F300	1 0 0 0 1	
2.180E-01	2.880E+01	15	D349	2 1 1 2 2	
1.759E-01	2.324E+01	20	B032	1 2 2 1 2	
2.210E-01	2.920E+01	20	D349	2 1 1 2 2	
1.589E-01	2.100E+01	20	F300	1 0 0 0 2	
8.477E-02	1.120E+01	21.5	P045	0 0 2 1 2	
2.226E-01	2.941E+01	25	B032	1 2 2 1 2	
2.260E-01	2.986E+01	25	D349	2 1 1 2 2	
1.709E-01	2.258E+01	25	G315	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N024	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N025	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N026	0 0 0 0 0	
1.853E-01	2.449E+01	25.1	N027	1 1 2 2 2	
1.918E-01	2.534E+01	27	D036	0 0 0 0 0	
2.233E-01	2.950E+01	27	D036	0 0 0 0 0	
2.777E-01	3.669E+01	29.80	B032	1 2 2 1 2	
2.604E+00	3.440E+02	98	F300	1 0 0 0 2	
1.817E-01	2.400E+01	ns	D072	0 0 0 0 1	
1.860E-01	2.457E+01	ns	M025	0 2 0 1 2	
1.774E-01	2.344E+01	rt	D021	0 0 1 1 2	

332. $C_4H_8N_2O_3.H_2O$

L-Asparagine monohydrate
Asparagine, monohydrate, L-

RN: 5794-13-8 **MP** (°C)**:** 234
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-01	2.902E+01	25	D041	1 0 0 0 2	
1.858E-01	2.790E+01	25	O316	1 0 1 2 2	
1.853E-01	2.781E+01	25	O316	1 0 1 2 2	
1.293E+00	1.941E+02	75	D041	1 0 0 0 2	

333. $C_4H_8N_4O_2$

N,N′-Dinitrosopiperazine
Dinitrosopiperazine

RN: 140-79-4 **MP** (°C)**:**
MW: 144.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	5.765E+00	24	D083	2 0 0 0 1	

334. C_4H_8O

2-Butyraldehyde
Butyraldehyde
Butyraldehyd
n-Butanal

RN: 123-72-8 **MP** (°C)**:** –96
MW: 72.11 **BP** (°C)**:** 75

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-01	3.568E+01	20	D041	1 0 0 0 1	
4.993E-01	3.600E+01	20	F300	1 0 0 0 1	
9.694E-01	6.990E+01	25	A049	1 0 0 0 2	
9.194E-01	6.629E+01	25	B060	2 0 1 1 1	
5.077E-01	3.661E+01	38	J020	2 2 2 1 1	

335. C_4H_8O

Ethyl vinyl ether
Aethyl-vinyl-aether

RN: 109-92-2 **MP** (°C)**:** –115.0
MW: 72.11 **BP** (°C)**:** 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	1.002E+01	37	E028	1 1 2 2 2	

336. C_4H_8O

Isobutyraldehyde
2-Methyl propanal

RN: 78-84-2 **MP** (°C)**:** –66
MW: 72.11 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	8.413E+01	20	M146	1 2 2 2 2	
1.234E+00	8.900E+01	25	A049	1 0 0 0 0	

337. C_4H_8O

Methyl ethyl ketone
Butanon-(2)

RN: 78-93-3 **MP** (°C)**:** –87
MW: 72.11 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
5.780E+00	4.168E+02	4	C423	0 0 0 0 0	
4.338E+00	3.128E+02	10	C423	0 0 0 0 0	
1.015E+00	7.322E+01	20	A075	1 0 0 0 1	

(*continued*)

337. C_4H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E+00	2.038E+02	20	D052	1 1 0 0 2	
2.922E+00	2.107E+02	20	E019	1 0 1 1 2	
2.399E+00	1.730E+02	20	F300	1 0 0 0 2	
2.977E+00	2.146E+02	20	G030	1 2 0 0 2	
5.020E+00	3.620E+02	20	P040	0 0 0 0 0	
2.931E+00	2.114E+02	25	A094	1 0 0 0 2	
3.302E+00	2.381E+02	25	A356	0 0 0 0 0	
2.931E+00	2.114E+02	25	B060	2 0 1 1 1	
3.732E+00	2.691E+02	25	C435	0 0 0 0 0	
3.130E+00	2.257E+02	25	F044	1 0 0 0 2	
2.824E+00	2.036E+02	25	G030	1 2 0 0 2	
2.657E+00	1.916E+02	25	J005	1 0 2 1 2	
6.112E+00	4.407E+02	25	K105	2 0 0 0 2	
2.912E+00	2.100E+02	25	M136	2 0 0 0 2	
2.912E+00	2.100E+02	25	M139	2 0 0 0 2	
2.720E+00	1.961E+02	25	N309	1 0 0 0 2	
2.756E+00	1.987E+02	25	O028	2 2 2 2 2	
2.556E+00	1.843E+02	25	P055	1 0 0 0 1	
2.774E+00	2.000E+02	25	R320	1 0 1 1 2	
2.690E+00	1.940E+02	30	G030	1 2 0 0 2	
1.703E+00	1.228E+02	30	R319	2 2 2 1 2	
2.900E+00	2.091E+02	35	A356	0 0 0 0 0	
2.969E+00	2.141E+02	35	C309	2 2 2 2 1	
2.538E+00	1.830E+02	38	J020	2 0 2 1 2	
7.726E-01	5.571E+01	40	A075	1 0 0 0 1	
2.723E+00	1.964E+02	45	A356	0 0 0 0 0	
2.615E+00	1.885E+02	45	C309	2 2 2 2 1	
6.257E+00	4.512E+02	45	K105	2 0 0 0 2	
6.855E-01	4.943E+01	60	A075	1 0 0 0 1	
6.319E+00	4.556E+02	60	K105	2 0 0 0 2	
6.352E-01	4.580E+01	70	A075	1 0 0 0 1	
3.453E+00	2.490E+02	70	P040	0 0 0 0 0	
2.219E+00	1.600E+02	90	F300	1 0 0 0 1	
3.627E+00	2.615E+02	100	P040	0 0 0 0 0	
6.844E+00	4.935E+02	140	P040	0 0 0 0 0	
3.334E+00	2.404E+02	ns	C309	2 2 2 2 1	
+1.89E+00	+1.36E+02	ns	S460	0 0 0 0 0	

338. C_4H_8O

Tetrahydrofuran
1,4-Epoxybutane
Butylene oxide

RN: 109-99-9 **MP** (°C)**:** –108.0
MW: 72.11 **BP** (°C)**:** 66.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E+00	3.243E+02	72.2	M347	2 2 2 1 2	
4.504E+00	3.248E+02	72.25	M347	2 2 2 1 2	

(*continued*)

338. C_4H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E+00	3.271E+02	72.3	M347	2 2 2 1 2	
4.251E+00	3.065E+02	73.4	M347	2 2 2 1 2	
4.019E+00	2.898E+02	75.4	M347	2 2 2 1 2	
3.678E+00	2.652E+02	78.6	M347	2 2 2 1 2	
3.595E+00	2.593E+02	78.9	M347	2 2 2 1 2	
3.378E+00	2.436E+02	83.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	87.9	M347	2 2 2 1 2	
3.217E+00	2.320E+02	89.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	92.9	M347	2 2 2 1 2	
3.042E+00	2.194E+02	102.5	M347	2 2 2 1 2	
3.042E+00	2.194E+02	110.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	119.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	127.8	M347	2 2 2 1 2	
3.595E+00	2.593E+02	132.9	M347	2 2 2 1 2	
3.998E+00	2.883E+02	136.1	M347	2 2 2 1 2	
4.067E+00	2.933E+02	136.5	M347	2 2 2 1 2	
4.617E+00	3.329E+02	137.1	M347	2 2 2 1 2	
6.934E+00	5.000E+02	rt	B066	0 2 0 0 2	

339. $C_4H_8O_2$

Ethyl acetate
Athylacetat
Essigsaeureaethyl ester

RN: 141-78-6 **MP** (°C)**:** –83
MW: 88.11 **BP** (°C)**:** 77

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.941E-01	8.759E+01	0	B108	1 2 0 1 1	
1.097E+00	9.666E+01	0	B108	1 2 0 1 2	
1.919E+00	1.691E+02	0	C423	0 0 0 0 0	
1.069E+00	9.420E+01	0	G062	1 2 2 2 2	
1.032E+00	9.091E+01	0	M088	2 0 0 0 1	
1.144E+00	1.008E+02	0	M111	1 0 1 1 2	
1.054E+00	9.290E+01	4	C423	0 0 0 0 0	
8.297E-01	7.310E+01	10	C423	0 0 0 0 0	
9.333E-01	8.223E+01	10	G062	1 2 2 2 2	
1.001E+00	8.817E+01	10	M111	1 0 1 1 2	
9.944E-01	8.762E+01	10.0	K079	1 0 0 0 2	
8.698E-01	7.664E+01	15	M088	2 0 0 0 1	
9.419E-01	8.299E+01	15	M111	1 0 1 1 2	
8.329E-01	7.339E+01	17.0	G101	1 2 1 1 2	
8.718E-01	7.681E+01	20	A016	1 2 1 1 2	
8.212E-01	7.236E+01	20	B108	1 2 0 1 1	
8.795E-01	7.749E+01	20	B108	1 2 0 1 2	
7.346E-01	6.472E+01	20	D052	1 1 0 0 2	
9.556E-01	8.419E+01	20	E002	1 0 0 0 2	
7.310E-01	6.441E+01	20	F001	1 0 1 2 2	

(*continued*)

339. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.932E-01	7.870E+01	20	F300	1 0 0 0 2	
8.920E-01	7.860E+01	20	M111	1 0 1 1 2	
7.300E-01	6.432E+01	20	M171	1 0 0 0 1	
7.732E-01	6.812E+01	20	M348	2 2 1 1 2	
9.200E-01	8.106E+01	20	S006	1 0 0 0 1	
8.778E-01	7.734E+01	20.0	K079	1 0 0 0 2	
8.708E-01	7.672E+01	20.40	A016	1 2 1 1 2	
8.417E-01	7.416E+01	25	A016	1 2 1 1 2	
9.084E-01	8.004E+01	25	A094	1 0 0 0 1	
8.243E-01	7.263E+01	25	A326	1 2 0 1 1	
5.396E-02	4.755E+00	25	B004	0 0 0 0 0	*sic*
9.084E-01	8.004E+01	25	B060	2 0 1 1 1	
9.180E-01	8.088E+01	25	B092	2 1 1 1 2	
9.080E-01	8.000E+01	25	B304	2 0 2 2 0	
7.321E-01	6.450E+01	25	C435	0 0 0 0 0	
8.988E-01	7.919E+01	25	D425	0 0 0 0 0	
7.810E-01	6.881E+01	25	G062	1 2 2 2 2	
7.977E-01	7.029E+01	25	L062	2 2 0 1 2	
9.847E-01	8.676E+01	25	L319	1 0 2 1 2	
8.485E-01	7.476E+01	25	M111	1 0 1 1 2	
8.310E-01	7.322E+01	25	P055	1 0 0 0 1	
8.222E-01	7.244E+01	25.0	K079	1 0 0 0 2	
8.436E-01	7.433E+01	25.10	A016	1 2 1 1 2	
7.653E-01	6.743E+01	27.0	G101	1 2 1 1 2	
7.603E-01	6.699E+01	27.5	G101	1 2 1 1 2	
8.124E-01	7.158E+01	30	A016	1 2 1 1 2	
8.115E-01	7.149E+01	30	A016	1 2 1 1 2	
7.524E-01	6.629E+01	30	M088	2 0 0 0 1	
8.124E-01	7.158E+01	30	M111	1 0 1 1 2	
7.524E-01	6.629E+01	30	S357	1 2 1 0 2	
7.889E-01	6.951E+01	30.0	K079	1 0 0 0 2	
7.800E-01	6.873E+01	34	A016	1 2 1 1 2	
7.810E-01	6.881E+01	35	A016	1 2 1 1 2	
7.791E-01	6.864E+01	35	M111	1 0 1 1 2	
8.170E-01	7.198E+01	37	E028	1 0 1 1 2	
7.077E-01	6.235E+01	37	G062	1 2 2 2 2	
7.444E-01	6.559E+01	37.0	K079	1 0 0 0 2	
7.425E-01	6.542E+01	38	J020	2 1 2 1 1	
7.574E-01	6.673E+01	39.90	A016	1 2 1 1 2	
7.504E-01	6.612E+01	40	A016	1 2 1 1 2	
7.395E-01	6.516E+01	40	B108	1 2 0 1 2	
7.524E-01	6.629E+01	40	M111	1 0 1 1 2	
6.696E-01	5.900E+01	40	M348	2 2 1 1 2	
7.278E-01	6.412E+01	40.0	K079	1 0 0 0 2	
6.465E-01	5.696E+01	50	G062	1 2 2 2 2	
6.722E-01	5.923E+01	50.0	K079	1 0 0 0 2	
5.907E-01	5.204E+01	55	M348	2 2 1 1 2	
7.820E-01	6.890E+01	60	B092	2 1 1 1 2	
6.790E-01	5.983E+01	70	A326	1 2 0 1 1	

(*continued*)

339. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.549E-01	4.889E+01	70	M348	2 2 1 1 2	
6.727E-01	5.927E+01	70.4	G101	1 2 1 1 1	
1.156E+00	1.018E+02	.0	K079	1 0 0 0 2	
1.600E-01	1.410E+01	ns	D348	0 0 0 0 0	

340. $C_4H_8O_2$

Methyl propionate
Methylester propanoic acid

RN: 554-12-1 **MP** (°C)**:** –87.0
MW: 88.11 **BP** (°C)**:** 79.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.083E+00	9.545E+01	-2.1	K079	1 0 0 0 2	
1.000E+00	8.811E+01	1.0	K079	1 0 0 0 2	
8.778E-01	7.734E+01	11.5	K079	1 0 0 0 2	
8.500E-01	7.489E+01	14.9	K079	1 0 0 0 2	
8.150E-01	7.181E+01	20	S006	1 0 0 0 2	
8.167E-01	7.195E+01	20.0	K079	1 0 0 0 2	
7.778E-01	6.853E+01	27.1	K079	1 0 0 0 2	
7.667E-01	6.755E+01	32.5	K079	1 0 0 0 2	
7.389E-01	6.510E+01	42.7	K079	1 0 0 0 2	

341. $C_4H_8O_2$

Isobutyric acid
Isobuttersaeure

RN: 79-31-2 **MP** (°C)**:** –47
MW: 88.11 **BP** (°C)**:** 153.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.931E+00	1.701E+02	15.2	P060	1 0 0 0 2	
1.931E+00	1.701E+02	15.2	P060	1 2 0 0 2	
4.171E+00	3.675E+02	17	P060	1 0 0 0 2	
4.171E+00	3.675E+02	17	P060	1 2 0 0 2	
2.619E+00	2.308E+02	17.7	H068	2 0 0 0 1	
1.892E+00	1.667E+02	20	D041	1 0 0 0 0	
1.894E+00	1.669E+02	20	F300	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 2 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 0 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.2	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.25	P060	1 0 0 0 2	
2.367E+00	2.085E+02	20.9	P060	1 0 0 0 2	
2.363E+00	2.082E+02	20.9	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 0 0 0 2	

(*continued*)

341. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.161E+00	2.785E+02	21.5	P060	1 2 0 0 2	
3.161E+00	2.785E+02	21.5	P060	1 0 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 2 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 0 0 0 2	
3.240E+00	2.855E+02	21.7	P060	1 2 0 0 2	
3.001E+00	2.644E+02	21.76	P060	1 0 0 0 2	
3.003E+00	2.645E+02	21.79	P060	1 0 0 0 2	
2.831E+00	2.495E+02	21.8	P060	1 2 0 0 2	
2.831E+00	2.495E+02	21.89	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 2 0 0 2	

342. $C_4H_8O_2$

3-Hydroxytetrahydrofuran
(*RS*)-3-Hydroxytetrahydrofuran
Tetrahydro-3-furanol
(±)-3-Hydroxytetrahydrofuran
3-Hydroxyoxolane

RN: 453-20-3 **MP** (°C)**:** <25
MW: 88.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.675E+00	5.000E+02	rt	B066	0 2 0 0 2	

343. $C_4H_8O_2$

Butyric acid
Buttersaeure
n-Butyric acid

RN: 107-92-6 **MP** (°C)**:** –7.9
MW: 88.11 **BP** (°C)**:** 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-02	2.593E+00	1.13	H068	2 0 0 0 1	
1.149E-01	1.012E+01	25	B004	0 0 0 0 0	

344. $C_4H_8O_2$

1,4-Dioxane
1,4-Dioxan
Dioxane

RN: 123-91-1 **MP** (°C)**:** 11.8
MW: 88.11 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>9.08E+00	>8.00E+02	25	B019	1 0 1 2 0	

345. $C_4H_8O_2$

Propyl formate
Ameisensaeure-propylester
Propyl methanoate
n-Propyl formate

RN: 110-74-7 **MP** (°C)**:** –93
MW: 88.11 **BP** (°C)**:** 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.222E-01	3.720E+01	-1.0	K079	1 0 0 0 2	
3.861E-01	3.402E+01	4.0	K079	1 0 0 0 2	
3.722E-01	3.280E+01	6.0	K079	1 0 0 0 2	
3.444E-01	3.035E+01	12.5	K079	1 0 0 0 2	
3.220E-01	2.837E+01	20	S006	1 0 0 0 2	
3.272E-01	2.883E+01	20.0	K079	1 0 0 0 2	
2.497E-01	2.200E+01	22	F300	1 0 0 0 1	
3.161E-01	2.785E+01	30.0	K079	1 0 0 0 2	
2.880E-01	2.537E+01	32.5	N014	0 0 0 0 0	
3.083E-01	2.717E+01	34.0	K079	1 0 0 0 2	
2.972E-01	2.619E+01	45.0	K079	1 0 0 0 2	

346. C_4H_9Br

Isobutyl bromide
1-Bromo-2-methylpropane

RN: 78-77-3 **MP** (°C)**:** –119
MW: 137.03 **BP** (°C)**:** 91.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	5.070E-01	18	F001	1 0 1 0 2	
3.722E-03	5.100E-01	18	F300	1 0 0 0 1	

347. C_4H_9Br

n-Butyl bromide
Bromobutane

RN: 109-65-9 **MP** (°C)**:** –112
MW: 137.03 **BP** (°C)**:** 101.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	5.892E-01	16	F001	1 0 1 0 2	
4.300E-03	5.892E-01	17	S006	1 0 0 0 1	
<1.46E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.500E-03	6.166E-01	25	K012	1 0 0 0 1	
6.340E-03	8.687E-01	25	M342	1 0 1 1 2	
4.434E-03	6.076E-01	30	G029	1 0 2 2 2	
4.500E-02	6.166E+00	ns	H307	0 0 0 0 0	

348. C_4H_9Cl
Isobutyl chloride
Isobutylchlorid
RN: 513-36-0 **MP** (°C)**:** –131
MW: 92.57 **BP** (°C)**:** 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	9.257E-01	12.5	F001	1 0 1 2 2	
9.722E-03	9.000E-01	12.50	F300	2 0 0 0 1	

349. C_4H_9Cl
n-Butyl chloride
1-Chlorobutane
RN: 109-69-3 **MP** (°C)**:** –123.0
MW: 92.57 **BP** (°C)**:** 78.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	6.665E-01	12.5	F001	1 0 1 0 2	
7.130E-02	6.600E+00	12.50	F300	1 0 0 0 1	
8.000E-03	7.406E-01	25	K012	1 0 0 0 0	
9.430E-03	8.729E-01	25	M342	1 0 1 1 2	
7.557E-03	6.995E-01	ns	N034	0 0 0 0 1	

350. C_4H_9Cl
sec-Butyl chloride
2-Chlorobutane
RN: 78-86-4 **MP** (°C)**:** –140
MW: 92.57 **BP** (°C)**:** 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.079E-02	9.990E-01	25	N034	1 0 0 0 0	

351. C_4H_9Cl
tert-Butyl chloride
2-Chloro-2-methylpropane
RN: 507-20-0 **MP** (°C)**:** –26.5
MW: 92.57 **BP** (°C)**:** 51.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.180E-02	7.572E+00	.99	C064	2 2 1 1 2	
6.620E-02	6.128E+00	5.00	C064	2 2 1 1 2	
3.110E-02	2.879E+00	14.90	C064	2 2 1 1 2	

352. C_4H_9I

Iodobutane
n-Butyl iodide
RN: 542-69-8 **MP** (°C)**:** –103
MW: 184.02 **BP** (°C)**:** 130.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.024E-01	17.5	F001	1 0 1 0 2	
1.100E-03	2.024E-01	17.5	S006	1 0 0 0 1	
1.100E-03	2.024E-01	20	M171	1 0 0 0 1	
1.700E-03	3.128E-01	25	K012	1 0 0 0 1	

353. C_4H_9NO

N,N-Dimethylacetamide
Acetdimethylamide
U-5954
RN: 127-19-5 **MP** (°C)**:** –20
MW: 87.12 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E+00	5.289E+02	4.50	C022	1 2 0 0 2	

354. C_4H_9NO

Butyramide
n-Butyramide
RN: 541-35-5 **MP** (°C)**:** 116
MW: 87.12 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E+00	1.708E+02	6	H059	0 0 0 0 0	
2.190E+00	1.908E+02	16	H059	0 0 0 0 0	
2.640E+00	2.300E+02	25	H059	0 0 0 0 0	

355. $C_4H_9NO_2$

γ-Aminobutyric acid
γ-Amino-buttersaeure
γ-Amino-*n*-butyric acid
RN: 56-12-2 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E+01	1.300E+03	25	M029	2 2 2 2 2	

356. $C_4H_9NO_2$
Propyl carbamate
n-Propyl carbamate
RN: 627-12-3 **MP** (°C)**:** 60
MW: 103.12 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E+00	2.001E+02	37	H006	1 2 2 1 2	

357. $C_4H_9NO_2$
DL-α-Aminobutyric acid
DL-2-Aminobutyric acid
RN: 2835-81-6 **MP** (°C)**:** 304
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E+00	2.188E+02	20	D041	1 0 0 0 1	
1.615E+00	1.665E+02	25	K031	2 1 2 1 2	

358. $C_4H_9NO_2$
β-Aminobutyric acid
β-Amino-*n*-butyric acid
RN: 2835-82-7 **MP** (°C)**:** 193
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+01	1.250E+03	25	M029	2 2 2 2 2	

359. $C_4H_9NO_2$
α-Aminoisobutyric acid
α-Amino-isobuttersaeure
α-Aminoisobutyric acid
2-Methylalanine
RN: 62-57-7 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E+00	1.371E+02	25	C018	0 0 0 0 0	
1.170E+00	1.206E+02	25	D041	1 0 0 0 2	
1.482E+00	1.528E+02	25	M029	2 2 2 2 2	
1.759E+00	1.814E+02	25	M097	2 2 2 2 2	

360. $C_4H_9NO_2$
1-Nitrobutane
Butane, 1-nitro-
RN: 627-05-4 **MP** (°C)**:** –81
MW: 103.12 **BP** (°C)**:** 152.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	3.609E+00	25	K012	1 0 0 0 1	

361. $C_4H_9NO_2$
N-Methylurethane
Ethyl methylaminoformate
Ethyl methylcarbamate
Ethyl *N*-methyl carbamate
Methyl urethane
N-Methylurethane
RN: 105-40-8 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.97E+00	+4.10E+02	ns	S460	0 0 0 0 0	

362. $C_4H_9NO_2$
α-Aminobutyric acid
2-Aminobutanoic acid
α-Amino-n-butyric acid
Butanoic acid
RN: 80-60-4 **MP** (°C)**:** 304
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	1.902E+02	25	A048	1 1 1 1 2	form A
1.624E+00	1.674E+02	25	A048	1 1 1 1 2	form B
1.800E+00	1.856E+02	25	C018	0 0 0 0 0	
1.800E+00	1.856E+02	25	E015	1 2 1 1 2	
2.041E+00	2.105E+02	25	M029	2 2 2 2 2	
1.852E+00	1.910E+02	35	A048	1 1 1 1 2	form A
1.771E+00	1.826E+02	35	A048	1 1 1 1 2	form B
1.931E+00	1.991E+02	45	A048	1 1 1 1 2	form A
1.917E+00	1.977E+02	45	A048	1 1 1 1 2	form B

363. $C_4H_9NO_3$
L-Threonine
Threonine
RN: 72-19-5 **MP** (°C)**:** 270
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.606E-01	9.060E+01	20	B032	1 2 2 1 2	
8.139E-01	9.695E+01	25	B032	1 2 2 1 2	
7.346E-01	8.751E+01	25	G315	0 0 0 0 0	
8.202E-01	9.770E+01	25.1	N024	0 0 0 0 0	
8.227E-01	9.800E+01	25.1	N026	0 0 0 0 0	
7.493E-01	8.925E+01	25.1	N027	1 1 2 2 2	
8.168E-01	9.730E+01	27	D036	0 0 0 0 0	
8.695E-01	1.036E+02	29.80	B032	1 2 2 1 2	

364. $C_4H_9NO_3$
DL-*allo*-Threonine
DL-Allothreonine
RN: 144-98-9 **MP** (°C)**:**
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E+00	1.220E+02	25	D041	1 0 0 0 2	
1.987E+00	2.366E+02	80	D041	1 0 0 0 2	

365. $C_4H_9NO_3$
DL-Threonine
(±)-Threonine
RN: 80-68-2 **MP** (°C)**:** 244
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E+00	1.674E+02	25	D041	1 0 0 0 2	
2.979E+00	3.548E+02	80	D041	1 0 0 0 1	

366. $C_4H_9NO_3$
Butyl nitrate
N-Butyl nitrate
RN: 928-45-0 **MP** (°C)**:**
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-03	7.743E-01	25	K012	1 0 0 0 1	

367. $C_4H_9N_3O_2$
Creatine
Kreatin
RN: 57-00-1 **MP** (°C)**:** 219
MW: 131.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.222E-02	1.078E+01	10	D041	1 0 0 0 2	
1.016E-01	1.332E+01	18	D041	1 0 0 0 2	
1.014E-01	1.330E+01	18	F300	1 0 0 0 2	

368. $C_4H_9O_5P$
γ-Phosphono-*n*-butyric acid
4-Phosphonobutyric acid
Phosphonic acid, (3-carboxypropyl)-
Butyric acid, 4-phosphono-
RN: 4378-43-2 **MP** (°C)**:**
MW: 168.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E+00	2.923E+02	0	N028	1 0 0 0 2	
2.068E+00	3.477E+02	20	N028	1 0 0 0 2	

369. C_4H_{10}
Isobutane
1,1-Dimethylethane
2-Methylpropane
Trimethylmethane
Purifrigor iso 3.5
R 600α
RN: 75-28-5 **MP** (°C)**:** –159
MW: 58.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~5.68E-03	~3.30E-01	17	F300	1 0 0 0 0	
8.413E-04	4.890E-02	25	M001	2 1 2 2 2	
8.413E-04	4.890E-02	25	M002	2 1 2 2 2	

370. C_4H_{10}

Butane
n-Butane
Diethyl
HC 600
Liquefied petroleum gas
R 600 (alkane)

RN: 106-97-8 **MP** (°C)**:** –138
MW: 58.12 **BP** (°C)**:** –0.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	1.824E-01	3	R063	0 0 0 0 0	
3.210E-03	1.866E-01	4	K031	2 1 2 1 2	
2.622E-03	1.524E-01	6	R063	0 0 0 0 0	
2.314E-03	1.345E-01	9	R063	0 0 0 0 0	
1.886E-03	1.096E-01	14	R063	0 0 0 0 0	
1.461E-03	8.492E-02	19.8	G058	1 0 0 0 2	
1.260E-03	7.324E-02	25	K031	2 1 2 1 2	
1.056E-03	6.140E-02	25	M001	2 1 2 2 2	
1.056E-03	6.140E-02	25	M002	2 1 2 2 2	
1.056E-03	6.140E-02	25	M040	1 0 0 1 2	
2.773E-02	1.612E+00	38	R078	0 0 0 0 0	
6.600E-04	3.836E-02	50	K031	2 1 2 1 2	
1.159E-01	6.735E+00	71	R078	0 0 0 0 0	
4.596E-01	2.671E+01	104	R078	0 0 0 0 0	
1.370E+00	7.965E+01	138	R078	0 0 0 0 0	

371. $C_4H_{10}NO_3PS$

Acephate
Orthene
Acetylphosphoramidothioic acid *O,S*-dimethyl ester

RN: 30560-19-1 **MP** (°C)**:** 85.5
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E+00	3.939E+02	rt	M161	0 0 0 0 1	

372. $C_4H_{10}N_2O$

N-Nitrosodiethylamine
Diethyl nitrosamine

RN: 55-18-5 **MP** (°C)**:**
MW: 102.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.062E+02	24	D083	2 0 0 0 2	

373. $C_4H_{10}O$

Methyl propyl ether
1-Methoxypropane

RN: 557-17-5 **MP** (°C)**:** <25
MW: 74.12 **BP** (°C)**:** 38.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.154E-01	5.303E+01	0	B002	2 1 1 2 2	
4.939E-01	3.661E+01	10	B002	2 1 1 2 2	
4.436E-01	3.288E+01	15	B002	2 1 1 2 2	
4.183E-01	3.101E+01	20	B002	2 1 1 2 2	
3.993E-01	2.960E+01	25	B002	2 1 1 2 2	

374. $C_4H_{10}O$

tert-Butyl alcohol
2-Methyl-2-propanol
tert-Butanol

RN: 75-65-0 **MP** (°C)**:** 25.6
MW: 74.12 **BP** (°C)**:** 82.41

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.712E-02	6.458E+00	79.40	B165	1 0 1 1 2	

375. $C_4H_{10}O$

n-Butyl alcohol
Butanol-(1)
n-Butanol
1-Butanol
Butyl alcohol
n-Butyl alcohol

RN: 71-36-3 **MP** (°C)**:** –90
MW: 74.12 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E+00	9.355E+01	0	E029	1 2 0 1 2	
1.176E+00	8.717E+01	0	M095	2 2 1 2 2	
1.176E+00	8.717E+01	5	H003	1 2 1 1 2	
1.077E+00	7.987E+01	10	E029	1 2 0 1 2	
1.104E+00	8.181E+01	10	H003	1 2 1 1 2	
6.015E+00	4.459E+02	13.0	J012	1 2 0 1 2	
1.024E+00	7.587E+01	15	H003	1 2 1 1 2	
1.034E+00	7.664E+01	15	M095	2 2 1 2 2	
9.190E-01	6.812E+01	18	F001	1 0 1 0 2	
8.634E-01	6.400E+01	18	F300	1 0 0 0 1	
7.396E-01	5.482E+01	20	A075	1 0 0 0 1	
9.762E-01	7.236E+01	20	D040	2 2 1 1 2	

(*continued*)

375. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.993E-01	7.407E+01	20	D052	1 1 0 0 0	
9.482E-01	7.029E+01	20	E029	1 2 0 1 2	
9.773E-01	7.244E+01	20	H003	1 2 1 1 2	
6.302E-01	4.671E+01	20	L084	1 1 1 1 1	
1.040E+00	7.709E+01	20	M312	1 0 0 0 1	
8.270E-01	6.130E+01	23	D063	1 0 1 2 2	
1.021E+00	7.567E+01	23.5	D063	1 0 0 2 2	
9.983E-01	7.400E+01	25	A049	1 0 1 0 0	
1.125E+00	8.341E+01	25	B019	1 0 1 2 0	
9.645E-01	7.149E+01	25	B060	2 0 1 1 1	
1.000E+00	7.412E+01	25	F044	1 0 0 0 0	EFG
8.708E-01	6.455E+01	25	F325	1 2 0 1 1	
9.200E-01	6.819E+01	25	G075	1 0 1 0 1	
9.237E-01	6.847E+01	25	H003	1 2 1 1 2	
9.307E-01	6.899E+01	25	H028	2 0 2 0 2	
1.070E+00	7.931E+01	25	K012	1 0 0 0 2	
9.700E-01	7.190E+01	25	K025	2 2 1 1 1	
8.867E-01	6.572E+01	25	L322	1 1 2 2 1	
8.904E-01	6.600E+01	25	M136	2 0 0 0 1	
8.904E-01	6.600E+01	25	M139	2 0 0 0 1	
8.826E-01	6.542E+01	25.0	P077	1 1 1 1 1	
8.234E-01	6.103E+01	26	O012	1 2 1 1 2	
8.826E-01	6.542E+01	27	R319	2 2 2 1 1	
5.976E+00	4.429E+02	29.82	J012	1 2 0 1 2	
8.944E-01	6.629E+01	30	D040	2 2 1 1 2	
8.897E-01	6.594E+01	30	E029	1 2 0 1 2	
8.920E-01	6.612E+01	30	F053	1 0 2 0 2	
8.920E-01	6.612E+01	30	H003	1 2 1 1 2	
8.838E-01	6.551E+01	30.0	H043	2 2 1 1 2	
8.625E-01	6.393E+01	35	H003	1 2 1 1 2	
9.061E-01	6.716E+01	38	J020	2 0 2 1 1	
8.471E-01	6.279E+01	38	M125	1 1 1 1 1	
5.933E-01	4.398E+01	40	A075	1 0 0 0 1	
8.353E-01	6.191E+01	40	D040	2 2 1 1 2	
8.495E-01	6.297E+01	40	E029	1 2 0 1 2	
8.353E-01	6.191E+01	40	H003	1 2 1 1 2	
8.234E-01	6.103E+01	45	M095	2 2 1 2 2	
8.293E-01	6.147E+01	50	E029	1 2 0 1 2	
8.186E-01	6.068E+01	50	H003	1 2 1 1 2	
7.756E-01	5.749E+01	50	O012	1 2 1 1 2	
5.837E+00	4.327E+02	58.50	J012	1 2 0 1 2	
5.064E-01	3.754E+01	60	A075	1 0 0 0 1	
8.258E-01	6.121E+01	60	E029	1 2 0 1 2	
8.258E-01	6.121E+01	60	H003	1 2 1 1 2	
5.064E-01	3.754E+01	70	A075	1 0 0 0 1	
8.436E-01	6.253E+01	70	E029	1 2 0 1 2	
8.850E-01	6.560E+01	70	F001	1 0 1 0 2	
8.507E-01	6.306E+01	70	H003	1 2 1 1 2	

(*continued*)

375. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-01	4.943E+01	75	L084	1 1 1 1 1	
8.590E-01	6.367E+01	75	M095	2 2 1 2 1	
8.708E-01	6.455E+01	80	E029	1 2 0 1 2	
9.460E-01	7.012E+01	80	F001	1 0 1 0 2	
8.696E-01	6.446E+01	80	H003	1 2 1 1 2	
9.412E-01	6.977E+01	90	E029	1 2 0 1 2	
1.054E+00	7.813E+01	90	F001	1 0 1 0 2	
9.762E-01	7.236E+01	90	M095	2 2 1 2 1	
1.084E+00	8.038E+01	97.90	H003	1 2 1 1 2	
1.101E+00	8.164E+01	98.3	R072	2 2 2 1 2	
4.900E+00	3.632E+02	100	E029	1 2 0 1 2	
1.228E+00	9.102E+01	100	F001	1 0 1 0 2	
1.204E+00	8.925E+01	105	M095	2 2 1 2 1	
1.342E+00	9.950E+01	110	E029	1 2 0 1 2	
1.473E+00	1.092E+02	110	F001	1 0 1 0 2	
1.523E+00	1.129E+02	114.50	H003	1 2 1 1 2	
1.600E+00	1.186E+02	116.90	H003	1 2 1 1 2	
1.805E+00	1.338E+02	120	E029	1 2 0 1 2	
2.223E+00	1.648E+02	123.30	H003	1 2 1 1 2	
2.890E+00	2.142E+02	124.80	H003	1 2 1 1 2	
2.567E+00	1.903E+02	125	E029	1 2 0 1 2	
3.334E+00	2.471E+02	125.10	H003	1 2 1 1 2	
3.148E+00	2.334E+02	125.20	H003	1 2 1 1 2	
9.307E-01	6.899E+01	ns	A406	0 0 0 0 1	
7.920E-01	5.871E+01	ns	D348	0 0 0 0 0	
9.744E-01	7.222E+01	ns	L003	0 0 2 1 2	
9.033E+00	6.695E+02	ns	M314	2 1 2 1 2	

376. $C_4H_{10}O$

Methyl isopropyl ether
2-Methoxypropane

RN: 598-53-8 **MP** (°C)**:** <25
MW: 74.12 **BP** (°C)**:** 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E+00	8.842E+01	10	B002	2 1 1 2 2	
1.068E+00	7.919E+01	15	B002	2 1 1 2 2	
9.295E-01	6.890E+01	20	B002	2 1 1 2 2	
8.234E-01	6.103E+01	25	B002	2 1 1 2 2	
8.437E-01	6.254E+01	ns	J300	0 0 0 0 0	

377. $C_4H_{10}O$

Isobutyl alcohol
2-Methyl-1-propanol

RN: 78-83-1 **MP** (°C)**:** –108
MW: 74.12 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E+00	1.001E+02	18	F001	1 0 1 2 2	
1.228E+00	9.100E+01	18	F300	1 0 0 0 0	
1.278E+00	9.471E+01	20	M146	1 2 2 2 2	
1.280E+00	9.488E+01	20	M312	1 0 0 0 1	
1.000E+00	7.416E+01	25	A037	2 2 2 2 2	
1.226E+00	9.091E+01	25	D052	1 1 0 0 2	
9.529E-01	7.063E+01	25	F050	1 0 0 0 1	
8.967E-01	6.647E+01	25	F317	2 1 1 1 2	
1.045E+00	7.749E+01	29.84	M114	2 2 1 1 1	
9.529E-01	7.063E+01	39.74	M114	2 2 1 1 1	
8.234E-01	6.103E+01	49.64	M114	2 2 1 1 1	
8.590E-01	6.367E+01	59.54	M114	2 2 1 1 1	
9.295E-01	6.890E+01	79.24	M114	2 2 1 1 1	
9.645E-01	7.149E+01	89.14	M114	2 2 1 1 1	
5.168E+00	3.831E+02	90.5	J017	1 0 1 2 2	
5.033E+00	3.730E+02	91.0	J017	1 0 1 2 2	
4.887E+00	3.622E+02	92.0	J017	1 0 1 2 2	
4.871E+00	3.610E+02	92.1	J017	1 0 1 2 2	
4.615E+00	3.421E+02	93.0	J017	1 0 1 2 2	
4.135E+00	3.065E+02	94.3	J017	1 0 1 2 2	
3.820E+00	2.832E+02	95.3	J017	1 0 1 2 2	
1.215E+00	9.008E+01	99.04	M114	2 2 1 1 1	
1.348E+00	9.991E+01	108.94	M114	2 2 1 1 2	
1.708E+00	1.266E+02	118.74	M114	2 2 1 1 2	
2.009E+00	1.489E+02	123.74	M114	2 2 1 1 2	
2.239E+00	1.660E+02	125.64	M114	2 2 1 1 2	
2.415E+00	1.790E+02	128.64	M114	2 2 1 1 2	
2.637E+00	1.955E+02	130.64	M114	2 2 1 1 2	
3.000E+00	2.224E+02	132.64	M114	2 2 1 1 2	
3.527E+00	2.614E+02	134.14	M114	2 2 1 1 2	
1.179E+00	8.740E+01	ns	L003	0 0 2 1 1	

378. $C_4H_{10}O$

Ethyl ether
Diaethylaether
Diethyl ether

RN: 60-29-7 **MP** (°C)**:** –116
MW: 74.12 **BP** (°C)**:** 34.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E+00	1.131E+02	–3.8	H002	2 0 0 1 2	
1.410E+00	1.045E+02	0	H002	1 0 0 1 2	
1.662E+00	1.232E+02	0	K077	1 2 2 2 2	average of 3
1.338E+00	9.920E+01	7.5	K077	1 2 2 2 2	

(*continued*)

378. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.263E+00	9.360E+01	8.5	K077	1 2 2 2 2	
1.118E+00	8.291E+01	10	H002	1 0 0 1 2	
1.115E+00	8.265E+01	10	K002	1 2 1 1 2	
1.105E+00	8.190E+01	12	K077	1 2 2 2 2	
9.796E-01	7.261E+01	15	F055	1 2 2 2 2	
1.133E+00	8.400E+01	15	F300	1 0 0 0 1	
9.893E-01	7.333E+01	15	H002	1 0 0 1 2	
9.843E-01	7.296E+01	15	K002	1 2 1 1 2	
8.430E+00	6.249E+02	15	M069	1 0 0 0 2	
1.137E+00	8.430E+01	15	T033	1 2 1 1 2	
1.029E+00	7.630E+01	16	K077	1 2 2 2 2	
8.837E-01	6.550E+01	19	K077	1 2 2 2 2	average
8.696E-01	6.446E+01	20	F055	1 2 2 2 2	
8.703E-01	6.451E+01	20	H002	1 0 0 1 2	
8.684E-01	6.437E+01	20	K002	1 2 1 1 2	
8.353E-01	6.191E+01	20	M345	2 1 1 1 1	
8.341E-01	6.183E+01	20	N038	1 0 0 1 2	
8.769E-03	6.500E-01	21	H337	1 0 1 0 2	*sic*
1.012E+00	7.502E+01	22	H072	1 0 1 1 2	
9.993E-01	7.407E+01	25	B019	1 0 1 2 0	
7.636E-01	5.660E+01	25	F055	1 2 2 2 2	
8.095E-01	6.000E+01	25	F300	1 0 0 0 1	
7.669E-01	5.684E+01	25	H002	1 0 0 1 2	
7.684E-01	5.696E+01	25	K002	1 2 1 1 2	
8.800E-01	6.523E+01	25	K012	1 0 0 0 1	
6.050E+00	4.484E+02	25	M069	1 0 0 0 2	
8.471E-01	6.279E+01	25	M345	2 1 1 1 1	
8.162E-01	6.050E+01	25	T033	1 2 1 1 2	
1.048E-02	7.770E-01	26	H337	1 0 1 0 2	*sic*
6.839E-01	5.069E+01	30	H002	1 0 0 1 2	
6.839E-01	5.069E+01	30	K002	1 2 1 1 2	
6.799E-01	5.040E+01	30	K077	1 2 2 2 2	
1.073E-02	7.950E-01	32	H337	1 0 1 0 2	*sic*
5.950E-01	4.410E+01	37	E022	1 0 1 1 0	
7.120E-01	5.278E+01	37	E028	1 0 1 1 2	
9.484E-03	7.030E-01	37	H337	1 0 1 0 2	*sic*
6.314E-01	4.680E+01	38	K077	1 2 2 2 2	
9.417E-03	6.980E-01	38.5	H337	1 0 1 0 2	*sic*
9.808E-03	7.270E-01	40	H337	1 0 1 0 2	*sic*
5.545E-01	4.110E+01	49	K077	1 2 2 2 2	
5.491E-01	4.070E+01	51.5	K077	1 2 2 2 2	
4.857E-01	3.600E+01	62.5	K077	1 2 2 2 2	
4.600E-01	3.410E+01	65	K077	1 2 2 2 2	
4.209E-01	3.120E+01	66.5	K077	1 2 2 2 2	
4.020E-01	2.980E+01	71	K077	1 2 2 2 2	
3.912E-01	2.900E+01	72	K077	1 2 2 2 2	
3.643E-01	2.700E+01	82	K077	1 2 2 2 2	
1.770E-01	1.312E+01	ns	D348	0 0 0 0 0	
9.412E-01	6.977E+01	ns	R028	0 0 0 0 0	
8.826E-01	6.542E+01	rt	B066	0 2 0 0 0	

379. $C_4H_{10}O$

sec-Butyl alcohol
DL-*sec*-Butyl alcohol
DL-Butanol-(2)
sec-DL-Butyl alcohol

RN: 78-92-2 **MP** (°C)**:** –114
MW: 74.12 **BP** (°C)**:** 99.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	1.929E+02	10.04	M119	2 2 2 2 2	
3.222E+00	2.388E+02	20	A070	1 2 1 0 2	
1.499E+00	1.111E+02	20	D052	1 1 0 0 0	
2.106E+00	1.561E+02	20	E019	1 0 1 1 2	
1.497E+00	1.110E+02	20	F300	1 0 0 0 2	
2.230E+00	1.653E+02	20	M112	2 2 1 1 2	
2.267E+00	1.681E+02	20.04	M119	2 2 2 2 2	
1.348E+00	9.991E+01	25	B019	1 0 1 2 0	
1.057E+00	7.834E+01	25	B060	2 0 1 1 1	
1.699E+00	1.260E+02	25	B165	1 0 1 1 1	
2.048E+00	1.518E+02	27.04	M119	2 2 2 2 2	
2.556E+00	1.894E+02	40	A070	1 2 1 0 2	
1.821E+00	1.349E+02	40	M112	2 0 1 1 2	
1.749E+00	1.297E+02	40.04	M119	2 2 2 2 2	
1.573E+00	1.166E+02	50.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	60	A070	1 2 1 0 2	
1.657E+00	1.228E+02	60	M112	2 0 1 1 2	
1.531E+00	1.135E+02	60.04	M119	2 2 2 2 2	
1.541E+00	1.143E+02	70.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	80	A070	1 2 1 0 2	
1.657E+00	1.228E+02	80	M112	2 0 1 1 2	
1.636E+00	1.213E+02	80.04	M119	2 2 2 2 2	
1.760E+00	1.304E+02	85	M112	2 0 1 1 2	
5.107E-02	3.786E+00	87.30	B165	1 0 1 1 2	
1.810E+00	1.342E+02	90.04	M119	2 2 2 2 2	
2.087E+00	1.547E+02	100.04	M119	2 2 2 2 2	
2.602E+00	1.929E+02	110.04	M119	2 2 2 2 2	
1.901E+00	1.409E+02	ns	L003	0 0 2 1 2	

380. $C_4H_{10}O_2S$

Diethyl sulfone
Diaethylsulfon

RN: 597-35-3 **MP** (°C)**:** 73
MW: 122.19 **BP** (°C)**:** 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E+00	1.350E+02	16	F300	1 0 0 0 2	

381. $C_4H_{10}O_4$
DL-Threitol
DL-1,2,3,4-Butanetetrol
RN: 6968-16-7 **MP** (°C)**:** 90
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.353E+00	8.980E+02	25	C346	0 0 0 0 0	

382. $C_4H_{10}O_4$
Erythritol
Erythrit
RN: 149-32-6 **MP** (°C)**:** 121.5
MW: 122.12 **BP** (°C)**:** 330

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.118E+00	3.808E+02	rt	D021	0 0 1 1 2	
4.995E+00	6.100E+02	rt	F300	0 0 0 0 2	

383. $C_4H_{10}S$
Ethyl sulfide
1,1′-Thiobisethane
Diethyl thioether
RN: 352-93-2 **MP** (°C)**:** –100
MW: 90.19 **BP** (°C)**:** 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	3.066E+00	25	K012	1 0 0 0 1	

384. $C_4H_{11}N$
sec-Butylamine
DL-*sec*-Butylamine
DL-*sec*-Butylamin
RN: 13952-84-6 **MP** (°C)**:**
MW: 73.14 **BP** (°C)**:** 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+00	1.120E+02	20	F300	1 0 0 0 2	

385. $C_4H_{11}N$

n-Butylamine
n-Butylamin
1-Aminobutane
RN: 109-73-9 **MP** (°C)**:** –50
MW: 73.14 **BP** (°C)**:** 78

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-02	2.384E+00	25	B004	0 0 0 0 0	

386. $C_4H_{11}NO_3$

Tromethamine
tris-(Hydroxymethyl)-amino-methan
tris-(Hydroxymethyl)-aminomethane
2-Amino-2-(hydroxymethyl)-1,3-propanediol
tris(Hydroxymethyl)methylamine
RN: 77-86-1 **MP** (°C)**:** 171.5
MW: 121.14 **BP** (°C)**:** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.564E+00	5.529E+02	15	E305	0 0 0 0 0	
5.766E+00	6.985E+02	25	E305	0 0 0 0 0	
7.160E+00	8.673E+02	35	E305	0 0 0 0 0	

387. $C_4H_{11}NO_8P_2$

Glyphosine
Polaris
N,*N*-bis(Phosphonomethyl)glycine
RN: 2439-99-8 **MP** (°C)**:**
MW: 263.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.427E-01	2.480E+02	20	M161	1 0 0 0 2	

388. C_4Cl_6

Hexachloro-1,3-butadiene
Hexachlorobutadiene
RN: 87-68-3 **MP** (°C)**:** –19
MW: 260.76 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	2.548E-03	20	C113	1 0 2 1 2	
1.917E-05	5.000E-03	20	M068	1 0 0 0 0	
~7.67E-06	~2.00E-03	20	M133	1 0 0 0 0	
1.240E-05	3.233E-03	25	B173	2 0 2 2 2	
7.668E-04	2.000E-01	ns	M061	0 0 0 0 1	

389. $C_5H_2Cl_3NO$
2,3,5-Trichloro-4-hydroxypyridine
Daxtrom
RN: 1970-40-7 **MP** (°C)**:** 216
MW: 198.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.871E-03	5.697E-01	25	M061	1 0 0 0 1	

390. $C_5H_2Cl_3NO$
3,5,6-Trichloro-2-pyridinol
3,5,6-Trichloropyridinol
Hydroxy-3,5,6-trichloropyridine
Pyridinone, 3,5,6-trichloro-
RN: 6515-38-4 **MP** (°C)**:**
MW: 198.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.200E-01	26.70	L095	2 2 1 1 2	
1.109E-03	2.200E-01	ns	K138	0 0 0 0 1	

391. $C_5H_3F_3N_2O_2$
5-Trifluoromethyl uracil
Trifluorothymine
RN: 54-20-6 **MP** (°C)**:**
MW: 180.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.451E-01	2.613E+01	25	S471	0 0 0 0 0	
1.492E-01	2.687E+01	25	S471	0 0 0 0 0	

392. $C_5H_4ClN_5$
2-Chloroadenine
1H-Purin-6-amine, 2-chloro-
6-Amino-2-chloropurine
2-Chloro-6-aminopurine
SQ 22982
RN: 1839-18-5 **MP** (°C)**:**
MW: 169.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-05	8.300E-03	25	A336	0 0 0 0 0	

393. $C_5H_4N_2O_4$
Orotic acid
Vitamin B13
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid
RN: 65-86-1 **MP** (°C)**:** 345.5
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-02	1.815E+00	18	B135	1 0 0 0 0	

394. $C_5H_4N_2O_4$
α,β-Imidazoledicarboxylic acid
4,5-Imidazoledicarboxylic acid
Imidazol-di-carbonsaeure-(4,5)
RN: 570-22-9 **MP** (°C)**:** 288
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.203E-03	5.000E-01	20	F300	1 0 0 0 1	
8.328E-03	1.300E+00	100	F300	1 0 0 0 1	

395. $C_5H_4N_2O_4$
5-Carboxyuracil
5-Uracilcarboxylic acid
2,4-Dihydroxypyrimidine-5-carboxylic acid
Uracil-carbonsaeure-(4)
RN: 23945-44-0 **MP** (°C)**:** 283
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	1.800E+00	20	F300	1 0 0 0 1	
7.000E-03	1.093E+00	20	N019	0 0 0 0 0	

396. $C_5H_4N_4$
Purine
7-Imidazo(4,5-d)pyrimidine
RN: 120-73-0 **MP** (°C)**:** 216
MW: 120.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.775E+00	3.333E+02	20	A018	1 0 1 1 0	
2.754E+00	3.308E+02	ns	R427	0 0 0 0 0	

397. $C_5H_4N_4O$
Hypoxanthine
Hypoxanthin
RN: 68-94-0 **MP** (°C)**:** 150dec
MW: 136.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-03	6.995E-01	19	D041	1 0 0 0 0	
5.143E-03	7.000E-01	23	F300	1 0 0 0 1	
5.290E-03	7.200E-01	25	A337	0 0 0 0 0	
~1.90E-03	~2.59E-01	39.99	T420	0 0 0 0 0	
1.042E-01	1.418E+01	100	D004	0 0 0 0 0	
1.080E-01	1.470E+01	100	F300	1 0 0 0 2	
5.359E-03	7.294E-01	c	D004	0 0 0 0 0	

398. $C_5H_4N_4O$
Allopurinol
1H-Pyrazolo(3,4-d)pyrimidin-4-ol
Lopurin
RN: 315-30-0 **MP** (°C)**:** >350
MW: 136.11 **BP** (°C)**:** 559.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-03	3.450E-01	15	C095	1 0 0 1 2	
3.673E-03	5.000E-01	22	B322	0 0 0 0 0	
3.673E-03	5.000E-01	22	B428	1 2 1 2 1	
3.526E-03	4.800E-01	25	B189	1 0 0 0 1	
4.180E-03	5.690E-01	25	C095	1 0 0 1 2	
6.502E-03	8.850E-01	35	C095	1 0 0 1 2	
7.964E-03	1.084E+00	40	C095	1 0 0 1 2	
3.526E-03	4.800E-01	ns	A351	0 0 0 0 0	
2.475E-03	3.369E-01	ns	B404	0 2 1 1 0	
5.730E-03	7.800E-01	ns	H067	0 0 0 0 0	
7.347E-04	1.000E-01	ns	K444	0 0 0 0 0	

399. $C_5H_4N_4O$
8-Hydroxypurine
9H-Purin-8-ol
RN: 51953-05-0 **MP** (°C)**:**
MW: 136.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.048E-02	4.149E+00	20	A022	1 0 0 0 0	

400. $C_5H_4N_4O_2$
Xanthine
2,6-Dioxopurine
1H-Purine-2,6-dione, 3,7-dihydro-
RN: 69-89-6 **MP** (°C)**:** >300
MW: 152.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.285E-03	4.998E-01	20	D041	1 0 0 0 0	
3.000E-04	4.563E-02	20.99	T418	0 0 0 0 0	
2.458E-04	3.739E-02	21	L015	1 0 1 1 2	
5.246E-04	7.980E-02	37	L015	1 0 1 1 2	
1.312E-02	1.996E+00	100	D041	1 0 0 0 0	

401. $C_5H_4N_4O_2.H_2O$
Xanthine (monohydrate)
RN: 69-89-6 **MP** (°C)**:** >150dec
MW: 170.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.082E-04	6.944E-02	c	D004	0 0 0 0 0	
3.916E-03	6.662E-01	h	D004	0 0 0 0 0	

402. $C_5H_4N_4O_3$
Uric acid
Harnsaeure
RN: 69-93-2 **MP** (°C)**:**
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-04	2.000E-02	0	M043	1 0 0 0 0	
7.110E-05	1.195E-02	2.6	M315	1 0 1 1 2	
1.029E-04	1.730E-02	5	R042	1 2 2 1 2	
1.050E-04	1.765E-02	9.3	M315	1 0 1 1 2	
2.379E-04	4.000E-02	10	M043	1 0 0 0 0	
1.326E-04	2.230E-02	14	B116	2 0 1 1 2	
1.190E-04	2.000E-02	20	D041	1 0 0 0 0	
3.569E-04	6.000E-02	20	M043	1 0 0 0 0	
6.610E-04	1.111E-01	22	M145	1 0 1 2 2	intrinsic
1.862E-04	3.130E-02	25	R042	1 2 2 1 2	
2.070E-04	3.480E-02	25.0	M315	1 0 1 1 2	
5.354E-04	9.000E-02	30	F300	1 0 0 0 2	
5.353E-04	8.999E-02	30	M043	1 0 0 0 0	
3.660E-04	6.153E-02	37.0	M315	1 0 1 1 2	
7.137E-04	1.200E-01	40	M043	1 0 0 0 1	
3.753E-04	6.310E-02	40	R042	1 2 2 1 2	
6.280E-04	1.056E-01	50.0	M315	1 0 1 1 2	
6.960E-04	1.170E-01	54	R042	1 2 2 1 2	
1.368E-03	2.299E-01	60	M043	1 0 0 0 1	

(*continued*)

402. $C_5H_4N_4O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-03	2.450E-01	70	F300	1 0 0 0 2	
2.319E-03	3.898E-01	80	M043	1 0 0 0 1	
2.974E-04	5.000E-02	100	D041	1 0 0 0 0	
4.961E-03	8.340E-01	100	F300	1 0 0 0 0	
3.686E-03	6.196E-01	100	M043	1 0 0 0 1	

403. $C_5H_4N_4O_3.2H_2O$

Uric acid (dihydrate)

RN: 69-93-2 **MP** (°C)**:**
MW: 204.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.620E-05	1.964E-02	2.6	M315	1 0 1 1 2	
1.420E-04	2.899E-02	9.3	M315	1 0 1 1 2	
3.390E-04	6.920E-02	25.0	M315	1 0 1 1 2	
6.560E-04	1.339E-01	37.0	M315	1 0 1 1 2	
1.440E-03	2.940E-01	50.0	M315	1 0 1 1 2	

404. $C_5H_4N_4S$

6-Mercaptopurine
6-Purinethiol
Mercaptopurine
Purine-6-thiol
Leukeran

RN: 50-44-2 **MP** (°C)**:**
MW: 152.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	4.565E-02	4.62	A034	1 1 2 2 0	EFG
8.148E-04	1.240E-01	25	N063	1 1 1 1 2	
4.500E-02	6.848E+00	29.87	A034	1 1 2 2 1	EFG
1.703E-03	2.591E-01	37	H046	1 1 1 1 2	
2.658E-03	4.045E-01	ns	N050	0 1 1 0 0	

405. $C_5H_4O_2$

Furfural
2-Furaldehyde
Furfurol

RN: 98-01-1 **MP** (°C)**:** –36
MW: 96.09 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.620E-01	7.322E+01	10	M099	1 2 0 1 1	
7.816E-01	7.510E+01	16	M099	1 2 0 1 2	
7.869E-01	7.561E+01	17	M099	1 2 0 1 2	
7.976E-01	7.664E+01	20	D052	1 1 0 0 0	

(*continued*)

405. $C_5H_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.972E-01	7.660E+01	20	F300	1 0 0 0 2	
7.976E-01	7.664E+01	20	M099	1 2 0 1 1	
7.620E-01	7.322E+01	25	C056	1 2 1 1 1	
8.197E-01	7.877E+01	25	C329	1 2 1 1 1	average
7.709E-01	7.407E+01	25	H338	2 2 1 2 2	
7.976E-01	7.664E+01	25	H340	0 0 0 0 0	
7.441E-01	7.149E+01	25	L062	2 2 1 2 1	
7.709E-01	7.407E+01	25	L320	2 2 1 2 1	
8.242E-01	7.919E+01	25	M099	1 2 0 1 1	
8.347E-01	8.021E+01	27	M099	1 2 0 1 2	
8.347E-01	8.021E+01	27.20	M099	1 2 0 1 2	
8.312E-01	7.987E+01	27.50	M099	1 2 0 1 2	
8.418E-01	8.088E+01	30	M099	1 2 0 1 1	
8.488E-01	8.156E+01	35	H338	2 2 1 2 2	
8.506E-01	8.173E+01	35	L320	2 2 1 2 1	
9.029E-01	8.676E+01	38	G050	1 0 2 1 1	
8.619E-01	8.282E+01	39.50	E037	1 2 2 2 2	
9.029E-01	8.676E+01	40	M099	1 2 0 1 1	
9.289E-01	8.925E+01	44	M099	1 2 0 1 2	
9.804E-01	9.420E+01	50	M099	1 2 0 1 2	
1.023E+00	9.829E+01	52	G050	1 0 2 1 2	
9.306E-01	8.942E+01	53.10	E037	1 2 2 2 2	
4.982E+00	4.787E+02	53.30	E037	1 2 2 2 2	
1.090E+00	1.047E+02	60	M099	1 2 0 1 2	
1.107E+00	1.063E+02	61	M099	1 2 0 1 2	
1.156E+00	1.111E+02	66	G050	1 0 2 1 2	
1.156E+00	1.111E+02	66	M099	1 2 0 1 2	
1.214E+00	1.166E+02	70	M099	1 2 0 1 2	
4.895E+00	4.703E+02	73.60	E037	1 2 2 2 2	
1.318E+00	1.266E+02	79	G050	1 0 2 1 2	
1.342E+00	1.289E+02	80	M099	1 2 0 1 2	
1.361E+00	1.307E+02	85.80	E037	1 2 2 2 2	
1.482E+00	1.424E+02	90	M099	1 2 0 1 2	
1.512E+00	1.453E+02	92	M099	1 2 0 1 2	
1.684E+00	1.618E+02	93	G050	1 0 2 1 2	
4.721E+00	4.536E+02	95.90	E037	1 2 2 2 2	
1.617E+00	1.554E+02	97.90	M099	1 2 0 1 2	

406. $C_5H_4O_2S$

3-Thenoic acid

Thiophen-carbonsaeure-(3)

RN: 88-13-1 **MP** (°C)**:** 137

MW: 128.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.355E-02	4.300E+00	25	F300	1 0 0 0 1	

407. $C_5H_4O_3$
2-Furoic acid
Furan-carbon-saeure-(2)
RN: 88-14-2 **MP** (°C)**:** 129.5
MW: 112.09 **BP** (°C)**:** 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.227E-01	2.496E+01	5.99	A341	0 0 0 0 0	
2.243E-01	2.514E+01	6.99	A341	0 0 0 0 0	
2.332E-01	2.614E+01	10.49	A341	0 0 0 0 0	
2.498E-01	2.799E+01	10.99	A341	0 0 0 0 0	
2.543E-01	2.851E+01	11.99	A341	0 0 0 0 0	
3.310E-01	3.710E+01	15	F300	1 0 0 0 2	
2.606E-01	2.921E+01	15.99	A341	0 0 0 0 0	
3.385E-01	3.794E+01	20.99	A341	0 0 0 0 0	
4.216E-01	4.725E+01	24.99	A341	0 0 0 0 0	
4.665E-01	5.229E+01	27.99	A341	0 0 0 0 0	
5.182E-01	5.808E+01	28.99	A341	0 0 0 0 0	
6.448E-01	7.227E+01	33.99	A341	0 0 0 0 0	
6.677E-01	7.484E+01	35.99	A341	0 0 0 0 0	
7.816E-01	8.761E+01	37.99	A341	0 0 0 0 0	
1.120E+00	1.256E+02	41.99	A341	0 0 0 0 0	
1.229E+00	1.378E+02	43.99	A341	0 0 0 0 0	
1.444E+00	1.618E+02	46.64	A341	0 0 0 0 0	
2.159E+00	2.420E+02	49.99	A341	0 0 0 0 0	
2.610E+00	2.926E+02	51.99	A341	0 0 0 0 0	
2.768E+00	3.103E+02	53.99	A341	0 0 0 0 0	
2.815E+00	3.155E+02	54.49	A341	0 0 0 0 0	
3.221E+00	3.610E+02	54.99	A341	0 0 0 0 0	
3.964E+00	4.443E+02	57.49	A341	0 0 0 0 0	
4.219E+00	4.729E+02	60.04	A341	0 0 0 0 0	
4.224E+00	4.735E+02	61.39	A341	0 0 0 0 0	
4.940E+00	5.537E+02	62.99	A341	0 0 0 0 0	
5.529E+00	6.197E+02	67.99	A341	0 0 0 0 0	
1.838E+00	2.060E+02	100	F300	1 0 0 0 2	

408. $C_5H_4O_3$
Isopyromucic acid
Isobrenzschleimsaeure
RN: 496-64-0 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-01	4.310E+01	0	F300	1 0 0 0 2	

409. $C_5H_5Cl_3N_2OS$
5-Ethoxy-3-trichloromethyl-1,2,4-thiadiazole
RN: 2593-15-9 **MP** (°C)**:**
MW: 247.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.732E-04	1.171E-01	ns	S460	0 0 0 0 0	

410. C_5H_5NO
3-Hydroxypyridine
3-Pyridinol
RN: 109-00-2 **MP** (°C)**:** 127.5
MW: 95.10 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.392E-01	3.226E+01	20	B050	1 0 0 0 0	

411. C_5H_5NO
4-Hydroxypyridine
4-Pyridinol
RN: 626-64-2 **MP** (°C)**:** 148
MW: 95.10 **BP** (°C)**:** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

412. C_5H_5NO
2-Hydroxypyridine
2-Pyridinol
RN: 72762-00-6 **MP** (°C)**:** 106
MW: 95.10 **BP** (°C)**:** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

413. $C_5H_5NO_2$
2,4-Dihydroxypyridine
3-Deazauracil
2,4-Pyridinediol
RN: 626-03-9 **MP** (°C)**:** 278
MW: 111.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.591E-02	6.211E+00	20	B050	1 0 0 0 0	

414. $C_5H_5N_3O$

Pyrazinamide
Pyrazine-2-carboxamide
Prazina

RN: 98-96-4 **MP** (°C)**:** 190
MW: 123.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-01	1.740E+01	25	N041	2 0 1 1 0	EFG
1.218E-01	1.500E+01	ns	K444	0 0 0 0 0	

415. $C_5H_5N_5$

Adenine
Adenin
6-Aminopurine
1H-Purin-6-amine
Adeninimine
Vitamin B4

RN: 73-24-5 **MP** (°C)**:** 363
MW: 135.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E-03	6.377E-01	17.5	S306	1 0 1 2 2	
6.328E-03	8.551E-01	18.8	S306	1 0 1 2 2	
6.494E-03	8.776E-01	19.2	S306	1 0 1 2 2	
7.382E-03	9.975E-01	19.7	S306	1 0 1 2 2	
7.000E-03	9.459E-01	20	C017	2 0 0 1 0	EFG
6.907E-03	9.333E-01	20.08	D307	0 0 0 0 0	
7.680E-03	1.038E+00	22.36	D307	0 0 0 0 0	
6.586E-03	8.900E-01	25	A337	0 0 0 0 0	
7.200E-03	9.729E-01	25	C416	2 1 1 1 1	
5.476E-03	7.400E-01	25	C437	0 0 0 0 0	Average
6.654E-03	8.992E-01	25	D041	1 0 0 0 0	
7.040E-03	9.513E-01	25	H061	0 0 0 0 0	
7.600E-03	1.027E+00	25	L080	2 1 2 1 2	
8.000E-03	1.081E+00	25	R039	0 0 0 0 0	
8.610E-03	1.163E+00	25.01	D307	0 0 0 0 0	
8.690E-03	1.174E+00	25.03	D307	0 0 0 0 0	
8.250E-03	1.115E+00	25.5	T008	1 1 2 2 2	
7.936E-03	1.072E+00	26.6	S306	1 0 1 2 2	
9.740E-03	1.316E+00	27.47	D307	0 0 0 0 0	
1.087E-02	1.469E+00	29.97	D307	0 0 0 0 0	
9.377E-03	1.267E+00	31.1	S306	1 0 1 2 2	
1.540E-02	2.081E+00	37	L042	2 0 2 2 2	pH 6.47
1.390E-02	1.878E+00	38	T008	1 1 2 2 2	
1.514E-02	2.045E+00	44.0	S306	1 0 1 2 2	
1.707E-02	2.307E+00	45.1	S306	1 0 1 2 2	
1.862E-02	2.516E+00	45.5	S306	1 0 1 2 2	

(*continued*)

415. $C_5H_5N_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-01	2.439E+01	100	D041	1 0 0 0 0	
6.808E-03	9.200E-01	c	D004	0 0 0 0 0	
1.805E-01	2.439E+01	h	D004	0 0 0 0 0	

416. $C_5H_5N_5O$

Guanine
2-Aminohypoxanthine
2-Amino-6-hydroxypurine

RN: 73-40-5 **MP** (°C)**:** >300
MW: 151.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	2.902E-03	15.02	D307	0 0 0 0 0	
6.000E-05	9.068E-03	20	C017	2 0 0 1 1	EFG
2.740E-05	4.141E-03	20.05	D307	0 0 0 0 0	
3.290E-05	4.972E-03	22.50	D307	0 0 0 0 0	
3.870E-05	5.849E-03	25.02	D307	0 0 0 0 0	
4.520E-05	6.831E-03	27.54	D307	0 0 0 0 0	
5.350E-05	8.085E-03	30.01	D307	0 0 0 0 0	
7.230E-05	1.093E-02	35.05	D307	0 0 0 0 0	
2.647E-04	4.000E-02	40	D041	1 0 0 0 0	
9.880E-05	1.493E-02	40.22	D307	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R424	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R427	0 0 0 0 0	

417. $C_5H_5N_5O$

Isoguanine
2-Hydroxy-6-aminopurine

RN: 3373-53-3 **MP** (°C)**:**
MW: 151.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.970E-04	6.000E-02	25	D041	1 0 0 0 0	
1.654E-03	2.499E-01	100	D041	1 0 0 0 1	

418. $C_5H_5N_5O_2$

2,8-Dioxyadenine
2,8-Dihydroxyadenine

RN: 30377-37-8 **MP** (°C)**:**
MW: 167.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-05	2.200E-03	25	B049	1 0 1 1 1	
8.556E-06	1.430E-03	37	P068	0 0 0 0 0	

419. C_5H_6

Cyclopentadiene
Pentolex
Pentole
Pyropentylene
R-Pentine
1,3-Cyclopentadiene

RN: 542-92-7 **MP** (°C)**:** –85
MW: 66.10 **BP** (°C)**:** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-02	6.764E-01	ns	S460	0 0 0 0 0	

420. $C_5H_6Cl_2N_2$

3-Methyluracil
2,4(1H,3H)-Pyrimidinedione, 3-methyl-
Uracil, 3-methyl-

RN: 608-34-4 **MP** (°C)**:**
MW: 165.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	2.000E+02	ns	B177	0 0 0 0 2	

421. $C_5H_6Cl_2N_2O_2$

Dantoin
1,3-Dichloro-5,5-dimethyl-2,4-imidazolidinedione
1,3-Dichloro-5,5-dimethylhydantoin

RN: 118-52-5 **MP** (°C)**:** 132
MW: 197.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.537E-03	4.998E-01	20	B080	1 0 1 1 0	
6.590E-03	1.298E+00	40	B080	1 0 1 1 1	

422. $C_5H_6N_2OS$

Methylthiouracil
6-Methyl-2-thiouracil

RN: 56-04-2 **MP** (°C)**:** 330
MW: 142.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-03	5.332E-01	25	G016	1 2 1 2 2	intrinsic
7.026E-03	9.990E-01	c	I310	0 0 0 0 0	
3.715E-03	5.283E-01	ns	R424	0 0 0 0 0	

423. $C_5H_6N_2OS$

5-Methyl-2-thiouracil
4(1H)-Pyrimidinone, 2,3-dihydro-5-methyl-2-thioxo-
2-Thiothymine
RN: 636-26-0 **MP** (°C)**:** 284
MW: 142.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.580E-03	5.090E-01	25	G016	1 2 1 2 2	intrinsic

424. $C_5H_6N_2O_2$

Thymine
2,4-Dihydroxy-5-methylpyrimidine
5-Methyluracil
RN: 65-71-4 **MP** (°C)**:** 316
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	2.775E+00	20	C017	2 0 0 1 1	EFG
2.379E-02	3.000E+00	23	F300	1 0 0 0 0	
3.552E-02	4.480E+00	25	D041	1 0 0 0 1	
2.780E-02	3.506E+00	25	H061	0 0 0 0 0	
3.030E-02	3.821E+00	25	L080	2 1 2 1 2	
2.860E-02	3.607E+00	25	R039	0 0 0 0 0	
2.740E-02	3.456E+00	25.5	T008	1 1 2 2 2	
3.500E-02	4.414E+00	30	L080	2 1 2 1 2	

425. $C_5H_6N_2O_2$

1-Methyluracil
2,4(1H,3H)-Pyrimidinedione, 1-methyl-
*N*1-Methyluracil
RN: 615-77-0 **MP** (°C)**:** 179
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.586E-01	2.000E+01	ns	B177	0 0 0 0 1	

426. $C_5H_6N_2O_4$

5-Carboxymethylhydantoin
Hydantoin of aspartic acid
RN: 5427-26-9 **MP** (°C)**:** 216
MW: 158.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-02	1.115E+01	ns	M025	0 2 0 1 2	

427. $C_5H_6O_2$
α-Angelica lactone
α-Angelica-lacton
RN: 591-12-8 **MP** (°C)**:** 18
MW: 98.10 **BP** (°C)**:** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-01	4.600E+01	15	F300	1 0 0 0 1	

428. $C_5H_6O_4$
Citraconic acid
Citraconsaeure
RN: 498-23-7 **MP** (°C)**:**
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.018E+00	7.830E+02	25	F300	1 0 0 0 2	

429. $C_5H_6O_4$
Mesaconic acid
Mesaconsaeure
RN: 498-24-8 **MP** (°C)**:** 204.5
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.022E-01	2.630E+01	18	F300	1 0 0 0 2	
4.241E+00	5.518E+02	100	F300	1 0 0 0 2	

430. $C_5H_6O_4$
Itaconic acid
Itaconsaeure
RN: 97-65-4 **MP** (°C)**:** 163
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.281E-01	5.570E+01	10	F300	1 0 0 0 2	
5.891E-01	7.664E+01	20	D041	1 0 0 0 1	
5.903E-01	7.680E+01	20	F300	1 0 0 0 2	

431. C_5H_6S

3-Methylthiophene

RN: 616-44-4 **MP** (°C)**:** –69
MW: 98.17 **BP** (°C)**:** 114 at 738 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-03	3.999E-01	ns	S460	0 0 0 0 0	

432. $C_5H_7NO_2$

Ethyl cyanoacetate
Cyanessigsaeure-aethyl ester

RN: 105-56-6 **MP** (°C)**:**
MW: 113.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.768E-01	2.000E+01	25	F300	1 0 0 0 0	
7.072E-01	8.000E+01	80	F300	1 0 0 0 0	

433. $C_5H_7NO_4S$

2,4-Thiazolidinedicarboxylic acid
Tidiacic acid
Tidiacic
TDCA

RN: 30097-06-4 **MP** (°C)**:**
MW: 177.18 **BP** (°C)**:** 524.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-02	7.619E+00	21	B414	1 0 0 1 1	

434. $C_5H_7N_2O_2$

6-Methyluracil
4-Methyl-uracil

RN: 626-48-2 **MP** (°C)**:** 318dec
MW: 127.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.506E-02	7.000E+00	22	F300	1 0 0 0 0	

435. $C_5H_7N_3O$

5-Methylcytosine
Mec

RN: 554-01-8 **MP** (°C)**:** 270
MW: 125.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.441E-01	4.306E+01	25	D041	1 0 0 0 1	

436. $C_5H_7N_3O_2$
Dimetridazole
1,2-Dimethyl-5-nitroimidazole
RN: 551-92-8 **MP** (°C)**:** 137–139
MW: 141.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.738E-02	9.509E+00	20	D344	0 0 0 0 0	
6.870E-02	9.696E+00	20	D344	0 0 0 0 0	

437. C_5H_8
Isoprene
2-Methyl-1,3-butadiene
RN: 78-79-5 **MP** (°C)**:** –120
MW: 68.12 **BP** (°C)**:** 34.07

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.425E-03	6.420E-01	25	M001	2 1 2 2 2	

438. C_5H_8
Cyclopentene
RN: 142-29-0 **MP** (°C)**:** –135
MW: 68.12 **BP** (°C)**:** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.411E-02	1.642E+00	24.8	L007	2 1 1 2 2	
7.854E-03	5.350E-01	25	M001	2 1 2 2 2	
2.411E-02	1.642E+00	25.1	L007	2 2 1 1 2	
2.562E-02	1.745E+00	34.8	L007	2 1 1 2 2	

439. C_5H_8
1-Pentyne
Pent-1-yne
RN: 627-19-0 **MP** (°C)**:** –106
MW: 68.12 **BP** (°C)**:** 40

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.305E-02	1.570E+00	25	M001	2 1 2 2 2	
1.154E-02	7.861E-01	25	M342	1 0 1 1 2	

440. C_5H_8
1,4-Pentadiene
Penta-1,4-diene
RN: 591-93-5 **MP** (°C)**:** –148
MW: 68.12 **BP** (°C)**:** 26

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.191E-03	5.580E-01	25	M001	2 1 2 2 2	

441. $C_5H_8BrNO_4$
5-Bromo-2-methyl-5-nitro-1,3-dioxane
Dioxane, 5-bromo-2-methyl-5-nitro-
Nibroxane
RN: 53983-00-9 **MP** (°C)**:** 72
MW: 226.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.695E-02	6.093E+00	25	L013	1 0 2 1 2	

442. $C_5H_8N_2O_2$
5,5′-Dimethylhydantoin
5,5-Dimethylhydantoin
5,5-Dimethyl-2,4-imidazolidinedione
5,5-Dimethylimidazolidine-2,4-dione
RN: 77-71-4 **MP** (°C)**:** 177
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.304E+02	37	F183	1 0 1 1 1	intrinsic

443. $C_5H_8N_2O_2$
5-Ethylhydantoin
Hydantoin of α-aminobutyric acid
RN: 15414-82-1 **MP** (°C)**:** 119
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-01	1.106E+02	ns	M025	0 2 0 1 2	

444. $C_5H_8N_4O_3S_2$

Methazolamide
Acetamide, *N*-[5-(aminosulfonyl)-3-methyl-1,3,4-thiadiazol-2(3H)-ylidene]-
N-(4-Methyl-2-sulfamoyl-D2-1,3,4-thiadiazolin-5-ylidene)acetamide
Neptazaneat
Metazolamide
Methenamide

RN: 554-57-4 **MP** (°C)**:** 213
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.725E-01	15	K024	1 2 1 1 1	
1.200E-02	2.835E+00	25	C415	1 0 0 1 0	
2.963E-03	7.000E-01	amb	L434	0 0 0 0 0	
1.481E-02	3.500E+00	ns	M032	0 0 0 0 2	
1.479E-02	3.495E+00	ns	R428	0 0 0 0 0	

445. $C_5H_8N_4O_{12}$

Pentaerythritol tetranitrate
Nitropentaerythritol
1,3-Propanediol, 2,2-*bis*[(nitrooxy)methyl]-, dinitrate (ester)

RN: 78-11-5 **MP** (°C)**:** 140
MW: 316.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.326E-06	2.000E-03	ns	M013	0 2 0 1 1	

446. C_5H_8O

Cyprethylene ether

RN: **MP** (°C)**:**
MW: 84.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.435E-02	7.937E+00	27	K058	1 0 1 1 0	

447. C_5H_8O

α-Methylcrotonaldehyde
α-Methyl-crotonaldehyd

RN: 623-36-9 **MP** (°C)**:**
MW: 84.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	2.000E+01	20	F300	1 0 0 0 1	

448. $C_5H_8O_2$
Ethyl acrylate
Ethyl propenoate
2-Propenoic acid ethyl ester
RN: 140-88-5 **MP** (°C)**:** –71
MW: 100.12 **BP** (°C)**:** 99.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.785E-01	1.787E+01	30	L096	1 2 0 2 2	

449. $C_5H_8O_2$
Methyl methacrylate
Methacrylic acid methyl ester
Methyl 2-methyl-2-propenoate
RN: 80-62-6 **MP** (°C)**:** –48
MW: 100.12 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.563E-01	1.565E+01	20	L096	1 2 0 2 2	

450. $C_5H_8O_2$
Acetylacetone
2,4-Pentanedione
Acetylaceton
RN: 123-54-6 **MP** (°C)**:** –23
MW: 100.12 **BP** (°C)**:** 140.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E+00	1.680E+02	19.0	N051	1 2 1 1 2	
1.703E+00	1.705E+02	19.5	N051	1 2 1 1 2	
1.089E+00	1.090E+02	20	F300	1 0 0 0 2	
1.706E+00	1.708E+02	25	B019	1 0 1 2 0	

451. $C_5H_8O_3$
Dimethylpyruvic acid
DL-Methyl-bernsteinsaeure
α-Ketoisovaleric acid
RN: 759-05-7 **MP** (°C)**:**
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E+00	4.006E+02	20	F300	1 0 0 0 2	

452. $C_5H_8O_3$
Levulinic acid
Laevulinsaeure
4-Oxopentanoic acid
3-Acetyl propionic acid
RN: 123-76-2 **MP** (°C)**:** 37.2
MW: 116.12 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.632E+00	5.378E+02	6.99	A340	0 0 0 0 0	
4.990E+00	5.795E+02	9.99	A340	0 0 0 0 0	
5.530E+00	6.422E+02	14.49	A340	0 0 0 0 0	
6.087E+00	7.068E+02	20.79	A340	0 0 0 0 0	
6.400E+00	7.431E+02	24.99	A340	0 0 0 0 0	
6.631E+00	7.700E+02	30.09	A340	0 0 0 0 0	

453. $C_5H_8O_4$
Methylsuccinic acid
Acide methylsuccinique
1,2-Propanedicarboxylic acid
RN: 498-21-5 **MP** (°C)**:** 117.5
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E+00	6.660E+02	15	M051	1 0 0 0 2	

454. $C_5H_8O_4$
Ethylmalonic acid
1,1-Propanedicarboxylic acid
Aethylmalonsaeure
Mono-ethyl malonate
Malonic acid monoethyl ester
Malonsaeure-monoaethyl ester
RN: 601-75-2 **MP** (°C)**:** 114
MW: 132.12 **BP** (°C)**:** 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E+00	3.460E+02	0	F300	1 0 0 0 2	
3.996E+00	5.280E+02	0	M051	1 0 0 0 2	
4.814E+00	6.360E+02	15	M051	1 0 0 0 2	
5.389E+00	7.120E+02	25	M051	1 0 0 0 2	
3.626E+00	4.790E+02	50	F300	1 0 0 0 2	
6.873E+00	9.080E+02	50	M051	1 0 0 0 2	

455. $C_5H_8O_4$
Dimethylmalonic acid
Dimethyl-malonsaeure
Dimethyl-propanedioic acid
RN: 595-46-0 **MP** (°C)**:** 192
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.812E-01	9.000E+01	13	F300	1 0 0 0 0	
1.968E+00	2.600E+02	100	F300	1 0 0 0 1	

456. $C_5H_8O_4$
Glutaric acid
Glutarsaeure
1,3-Propanedicarboxylic acid
RN: 110-94-1 **MP** (°C)**:** 96.5
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.272E+00	3.002E+02	0	F300	1 0 0 0 2	
3.247E+00	4.290E+02	0	L041	1 0 0 1 2	
2.410E+00	3.183E+02	3.40	A031	1 2 2 2 2	
2.650E+00	3.501E+02	5.99	A341	0 0 0 0 0	
2.764E+00	3.651E+02	7.99	A341	0 0 0 0 0	
3.127E+00	4.131E+02	10.40	A031	1 2 2 2 2	
2.909E+00	3.843E+02	10.99	A341	0 0 0 0 0	
3.213E+00	4.245E+02	12.99	A341	0 0 0 0 0	
3.433E+00	4.536E+02	14	A031	1 2 2 2 0	
4.443E+00	5.870E+02	15	L041	1 0 0 1 2	
4.443E+00	5.870E+02	15	M051	1 0 0 0 2	
3.521E+00	4.652E+02	15.99	A341	0 0 0 0 0	
3.674E+00	4.854E+02	17.99	A341	0 0 0 0 0	
3.861E+00	5.100E+02	18	A031	1 2 2 2 2	
3.816E+00	5.041E+02	19.99	A341	0 0 0 0 0	
2.954E+00	3.902E+02	20	D041	1 0 0 0 1	
4.837E+00	6.390E+02	20	L041	1 0 0 1 2	
2.952E+00	3.900E+02	20	M171	1 0 0 0 2	
1.340E+00	1.770E+02	20	S006	1 0 0 0 2	
4.278E+00	5.652E+02	23.90	A031	1 2 2 2 2	
4.088E+00	5.401E+02	24.99	A341	0 0 0 0 0	
4.653E+00	6.148E+02	28.30	A031	1 2 2 2 2	
4.394E+00	5.805E+02	28.99	A341	0 0 0 0 0	
4.503E+00	5.949E+02	30.99	A341	0 0 0 0 0	
4.642E+00	6.133E+02	33.99	A341	0 0 0 0 0	
6.033E+00	7.970E+02	35	L041	1 0 0 1 2	
4.796E+00	6.336E+02	36.99	A341	0 0 0 0 0	
4.894E+00	6.466E+02	38.99	A341	0 0 0 0 0	
5.096E+00	6.732E+02	42.99	A341	0 0 0 0 0	
5.131E+00	6.779E+02	43.99	A341	0 0 0 0 0	
5.143E+00	6.795E+02	44.99	A341	0 0 0 0 0	

(*continued*)

456. $C_5H_8O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.246E+00	6.930E+02	46.99	A341	0 0 0 0 0	
5.341E+00	7.057E+02	49.99	A341	0 0 0 0 0	
7.244E+00	9.570E+02	50	L041	1 0 0 1 2	
5.470E+00	7.227E+02	54.49	A341	0 0 0 0 0	
5.640E+00	7.451E+02	55.99	A341	0 0 0 0 0	
5.713E+00	7.548E+02	58.99	A341	0 0 0 0 0	
5.729E+00	7.569E+02	61.09	A341	0 0 0 0 0	
5.890E+00	7.782E+02	62.99	A341	0 0 0 0 0	
4.032E+00	5.327E+02	65	F300	1 0 0 0 2	
8.462E+00	1.118E+03	65	L041	1 0 0 1 2	
6.038E+00	7.977E+02	68.99	A341	0 0 0 0 0	
4.081E+00	5.392E+02	rt	H431	0 0 0 0 0	

457. $C_5H_9BrO_2$

α-Bromo-methyl-ethyl-acetate
Ethyl DL-α-bromopropionate
Propanoic acid, 2-bromo-, ethyl ester
Ethyl DL-2-bromopropionate

RN: 535-11-5 **MP** (°C)**:**
MW: 181.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-01	5.033E+01	ns	F057	0 2 2 2 1	

458. $C_5H_9BrO_2$

α-Ethyl-β-bromo-propionic ureide

RN: **MP** (°C)**:**
MW: 181.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-01	3.855E+01	ns	F056	0 2 2 2 1	

459. $C_5H_9NO_2$

DL-Proline
Pyrrolidine-2-carboxylic acid

RN: 609-36-9 **MP** (°C)**:** 208
MW: 115.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.217E+01	1.401E+03	20	J303	0 0 0 0 0	
1.146E+01	1.319E+03	25	J303	0 0 0 0 0	
1.425E+01	1.641E+03	40	J303	0 0 0 0 0	
1.708E+01	1.967E+03	50	J303	0 0 0 0 0	
2.082E+01	2.397E+03	60	J303	0 0 0 0 0	

460. $C_5H_9NO_2$
L-Proline
2-Pyrrolidinecarboxylic acid
RN: 147-85-3 **MP** (°C)**:**
MW: 115.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E+00	6.188E+02	25	D041	1 0 0 0 2	
6.653E+00	7.660E+02	27	D036	0 0 0 0 0	
6.123E+00	7.050E+02	65	D041	1 0 0 0 2	
6.691E+00	7.704E+02	99.99	P349	0 0 0 0 0	

461. $C_5H_9NO_2S$
2-Methylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-methyl-
Thiazolidine-4-carboxylic acid, 2-methyl-
RN: 4165-32-6 **MP** (°C)**:** 174-175
MW: 147.20 **BP** (°C)**:** 333.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-01	3.091E+01	21	B414	1 0 0 1 1	partial decomposition

462. $C_5H_9NO_3$
L-Hydroxyproline
trans-4-Hydroxy-L-proline
L-4-hydroxyproline
(4*S*)-4-Hydroxy-L-proline
RN: 51-35-4 **MP** (°C)**:**
MW: 131.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.158E+00	4.141E+02	99.99	P349	0 0 0 0 0	

463. $C_5H_9NO_3$
Formyl-α-aminobutyric acid
Butanoic acid, 2-(formylamino)-
RN: 106873-99-8 **MP** (°C)**:**
MW: 131.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-01	3.357E+01	25	M024	1 2 0 1 2	
2.560E-01	3.357E+01	ns	M025	0 2 0 1 2	

464. $C_5H_9NO_4$

D-Glutamic acid
D-2-Aminoglutaric acid
RN: 6893-26-1 **MP** (°C)**:** 201
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-02	3.439E+00	0	D018	2 2 2 1 2	
2.303E-02	3.388E+00	0	M043	1 0 0 0 1	
3.381E-02	4.975E+00	10	M043	1 0 0 0 1	
1.004E-01	1.478E+01	20	D041	1 0 0 0 1	
4.859E-02	7.149E+00	20	M043	1 0 0 0 1	
4.472E-02	6.580E+00	21	P045	1 0 2 1 2	
5.981E-02	8.800E+00	25	D018	2 2 2 1 2	
6.729E-02	9.901E+00	30	M043	1 0 0 0 1	
1.004E-01	1.478E+01	40	M043	1 0 0 0 1	
1.481E-01	2.179E+01	50	D018	2 2 2 1 2	
2.107E-01	3.101E+01	60	M043	1 0 0 0 1	
4.148E-01	6.103E+01	80	M043	1 0 0 0 1	
8.347E-01	1.228E+02	100	M043	1 0 0 0 2	
5.850E-02	8.607E+00	ns	M025	0 2 0 1 2	

465. $C_5H_9NO_4$

DL-Glutamic acid
DL-2-Aminoglutaric acid
RN: 617-65-2 **MP** (°C)**:** 194
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-02	8.241E+00	0	D018	2 2 2 1 2	
4.850E-02	7.136E+00	4.99	A405	2 0 1 1 2	
5.990E-02	8.813E+00	9.99	A405	2 0 1 1 2	
6.300E-02	9.269E+00	14.99	A405	2 0 1 1 2	
8.840E-02	1.301E+01	20.99	A405	2 0 1 1 2	
9.370E-02	1.379E+01	24.99	A405	2 0 1 1 2	
1.750E-01	2.575E+01	25	D018	2 2 2 1 2	
1.368E-01	2.013E+01	25	D041	1 0 0 0 2	
1.075E-01	1.582E+01	29.99	A405	2 0 1 1 2	
1.414E-01	2.080E+01	34.99	A405	2 0 1 1 2	
1.684E-01	2.478E+01	39.99	A405	2 0 1 1 2	
2.016E-01	2.966E+01	44.99	A405	2 0 1 1 2	
2.699E-01	3.971E+01	49.99	A405	2 0 1 1 2	
5.131E-01	7.549E+01	50	D018	2 2 2 1 2	
3.502E-01	5.153E+01	54.99	A405	2 0 1 1 2	
3.959E-01	5.825E+01	59.99	A405	2 0 1 1 2	
4.772E-01	7.021E+01	64.99	A405	2 0 1 1 2	
5.621E-01	8.270E+01	69.99	A405	2 0 1 1 2	
6.709E-01	9.871E+01	71.99	A405	2 0 1 1 2	
7.289E-01	1.072E+02	74.99	A405	2 0 1 1 2	
7.206E-01	1.060E+02	75	D041	1 0 0 0 2	

466. $C_5H_9NO_4$
L-Glutamic acid
L-2-Aminoglutaric acid
L(+)-Glutaminsaeure
Glutamic acid
L(+) Glutaminic acid
RN: 56-86-0 **MP** (°C)**:** 250
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.866E-02	7.160E+00	20	B032	1 2 2 1 2	
4.486E-02	6.600E+00	21	F302	1 0 0 0 1	
5.825E-02	8.570E+00	25	B032	1 2 2 1 2	
5.822E-02	8.566E+00	25	D041	1 0 0 0 2	
5.845E-02	8.600E+00	25	F300	1 0 0 0 1	
7.262E-02	1.068E+01	25	G315	0 0 0 0 0	
5.614E-02	8.260E+00	27	D036	0 0 0 0 0	
6.980E-02	1.027E+01	29.80	B032	1 2 2 1 2	
1.454E-01	2.140E+01	50	F300	1 0 0 0 2	
3.562E-01	5.240E+01	75	D041	1 0 0 0 2	
3.561E-01	5.240E+01	75	F300	1 0 0 0 2	
8.346E-01	1.228E+02	100	F300	1 0 0 0 2	
4.078E-02	6.000E+00	ns	D072	0 0 0 0 0	
5.802E-02	8.537E+00	rt	H431	0 0 0 0 0	

467. C_5H_{10}
Cyclopentane
Pentamethylene
Exxsol cyclopentane S
Zeonsolv HP
RN: 287-92-3 **MP** (°C)**:** –94.4
MW: 70.14 **BP** (°C)**:** 49.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.826E-03	3.385E-01	4.8	L007	2 2 1 2 2	
4.826E-03	3.385E-01	5.1	L007	2 1 1 1 2	
4.870E-03	3.416E-01	14.8	L007	2 2 1 2 2	
4.870E-03	3.416E-01	15.2	L007	2 1 1 1 2	
4.873E-03	3.418E-01	24.8	L007	2 2 1 2 2	
2.338E-03	1.640E-01	25	G313	2 1 1 2 2	
2.281E-03	1.600E-01	25	K119	1 0 0 0 2	
2.224E-03	1.560E-01	25	M001	2 1 2 2 2	
2.224E-03	1.560E-01	25	M002	2 1 2 2 2	
2.281E-03	1.600E-01	25.0	P051	2 1 1 2 2	
2.281E-03	1.600E-01	25.00	P007	2 1 2 2 2	
4.873E-03	3.418E-01	25.1	L007	2 1 1 1 2	
5.252E-03	3.684E-01	34.8	L007	2 2 1 2 2	
5.252E-03	3.684E-01	35.2	L007	2 1 1 1 2	
2.324E-03	1.630E-01	40.1	P051	2 1 1 2 2	

(*continued*)

467. C_5H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-03	1.630E-01	40.10	P007	2 1 2 2 2	
4.867E-03	3.414E-01	44.8	L007	2 2 1 2 2	
2.566E-03	1.800E-01	55.7	P051	2 1 1 2 2	
2.566E-03	1.800E-01	55.70	P007	2 1 2 2 2	
4.220E-03	2.960E-01	99.1	P051	2 1 1 2 2	
4.220E-03	2.960E-01	99.10	P007	2 1 2 2 2	
5.304E-03	3.720E-01	118.0	P051	2 1 1 2 2	
5.304E-03	3.720E-01	118.00	P007	2 1 2 2 2	
8.712E-03	6.110E-01	137.3	P051	2 1 1 2 2	
8.712E-03	6.110E-01	137.30	P007	2 1 2 2 2	
1.129E-02	7.920E-01	153.1	P051	2 1 1 2 2	
1.129E-02	7.920E-01	153.10	P007	2 1 2 2 2	
2.224E-03	1.560E-01	ns	H123	0 0 0 0 0	

468. C_5H_{10}

3-Methyl-1-butene
2-Methyl-3-butene
3,3-Dimethylpropene
Isopropylethylene

RN: 563-45-1 **MP** (°C)**:** –168
MW: 70.14 **BP** (°C)**:** 20

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-03	1.300E-01	25	M001	2 1 2 2 2	

469. C_5H_{10}

2-Pentene
1-Methyl-2-ethylethylene
sym-Methylethylethylene
β-Amylene
β-*n*-Amylene
3-Pentene

RN: 109-68-2 **MP** (°C)**:** –136
MW: 70.14 **BP** (°C)**:** 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-03	2.030E-01	25	M001	2 1 2 2 2	

470. C_5H_{10}
1-Pentene
Propylethylene
α-*n*-Amylene
1-Methyl-3-butene
RN: 109-67-1 **MP** (°C)**:** –165
MW: 70.14 **BP** (°C)**:** 30.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-03	1.830E-01	23	C332	0 0 0 0 0	
2.110E-03	1.480E-01	25	M001	2 1 2 2 2	

471. $C_5H_{10}Cl_3O_3P$
Diethyl trichloromethyl phosphonate
Phosphonic acid, (trichloromethyl)-, diethyl ester
Ro 3-0658
RN: 866-23-9 **MP** (°C)**:**
MW: 255.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-02	4.500E+00	25	B070	1 2 0 1 1	

472. $C_5H_{10}N_2O$
N-Nitrosopiperidine
Pyridine, hexahydro-*N*-nitroso
NPIP
RN: 100-75-4 **MP** (°C)**:** <25
MW: 114.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	7.648E+01	24	D083	2 0 0 0 1	

473. $C_5H_{10}N_2O_2S$
Methomyl
Nudrin
Lannate
RN: 16752-77-5 **MP** (°C)**:** 78.5
MW: 162.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-01	5.800E+01	25	M161	1 0 0 0 1	

474. $C_5H_{10}N_2O_3$
Glycolylglycineamide
RN: **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E+00	8.506E+02	25	M008	1 0 0 0 2	

475. $C_5H_{10}N_2O_3$
Glycyl-L-alanine
Glycylalanine
RN: 3695-73-6 **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E+00	6.986E+02	24.99	B441	0 0 0 0 0	

476. $C_5H_{10}N_2O_3$
D-Glutamine
D-2-Aminoglutaramic acid
RN: 5959-95-5 **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.910E-01	4.253E+01	ns	M025	0 2 0 1 2	

477. $C_5H_{10}N_2O_3$
L-Glutamine
L(+)-Glutamin
L(+)-Glutamine
Glutamine
RN: 56-85-9 **MP** (°C)**:** 185
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.184E-01	1.730E+01	0	F300	1 0 0 0 2	
2.378E-01	3.475E+01	18	D041	1 0 0 0 1	
2.444E-01	3.572E+01	20	B032	1 2 2 1 2	
2.829E-01	4.135E+01	25	B032	1 2 2 1 2	
2.789E-01	4.077E+01	25	D041	1 0 0 0 2	
2.701E-01	3.948E+01	25	G315	0 0 0 0 0	
5.891E-02	8.610E+00	25	J303	0 0 0 0 0	
2.997E-01	4.380E+01	25.1	N024	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N025	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N026	0 0 0 0 0	

(*continued*)

477. $C_5H_{10}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.821E-01	4.123E+01	25.1	N027	1 1 2 2 2	
2.737E-01	4.000E+01	27	D036	0 0 0 0 0	
3.285E-01	4.801E+01	29.80	B032	1 2 2 1 2	
3.154E-01	4.610E+01	30	F300	1 0 0 0 2	
1.002E-01	1.464E+01	40	J303	0 0 0 0 0	
2.135E-01	3.120E+01	60	J303	0 0 0 0 0	

478. $C_5H_{10}N_2S_2$

Dazomet
3,5-Dimethyl-1,2,3,5-tetrahydro-1,3,5-thiadiazinethione-2
Thiazone
Thiazon

RN: 533-74-4 **MP** (°C)**:** 106.5
MW: 162.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.386E-03	1.199E+00	25	M061	1 0 0 0 1	
1.169E-02	1.896E+00	30	B185	0 0 0 0 0	
7.395E-03	1.200E+00	30	M161	1 0 0 0 1	

479. $C_5H_{10}N_6O_2$

Dinitrosopentamethylenetetramine
3,7-Dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane

RN: 101-25-7 **MP** (°C)**:** 207
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.318E-02	9.901E+00	ns	I313	0 0 0 0 0	

480. $C_5H_{10}O$

Methy propyl ketone
Methyl propyl ketone
2-Pentanone
Pentan-2-one

RN: 107-87-9 **MP** (°C)**:** –78
MW: 86.13 **BP** (°C)**:** 100.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.870E-01	7.640E+01	10	G032	1 2 1 1 2	
6.520E-01	5.616E+01	20	G030	1 2 0 0 2	
5.000E-01	4.307E+01	20	M312	1 0 0 0 1	
6.799E-01	5.857E+01	25	A356	0 0 0 0 0	
4.786E-01	4.123E+01	25	B060	2 0 1 1 1	

(*continued*)

480. $C_5H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-01	6.697E+01	25	C333	0 0 0 0 0	
7.000E-01	6.029E+01	25	F044	1 0 0 0 1	
6.063E-01	5.222E+01	25	G030	1 2 0 0 2	
6.572E-01	5.660E+01	25	P055	1 0 0 0 2	
5.718E-01	4.925E+01	30	G030	1 2 0 0 2	
6.300E-01	5.426E+01	30	G032	1 2 1 1 2	
5.806E-01	5.001E+01	35	A356	0 0 0 0 0	
6.799E-01	5.857E+01	35	C333	0 0 0 0 0	
5.302E-01	4.567E+01	45	A356	0 0 0 0 0	
6.799E-01	5.857E+01	45	C333	0 0 0 0 0	
5.150E-01	4.436E+01	50	G032	1 2 1 1 2	
5.302E-01	4.567E+01	55	A356	0 0 0 0 0	
5.806E-01	5.001E+01	55	C333	0 0 0 0 0	

481. $C_5H_{10}O$

Valeraldehyde
n-Valeraldehyde
Valeral
n-Pentanal

RN: 110-62-3 **MP** (°C)**:** –92
MW: 86.13 **BP** (°C)**:** 103

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-01	1.170E+01	25	A049	1 0 0 0 2	
2.100E-01	1.809E+01	25	K012	1 0 0 0 1	

482. $C_5H_{10}O$

Tetrahydropyran
Pentamethylene oxide

RN: 142-68-7 **MP** (°C)**:** –49.2
MW: 86.13 **BP** (°C)**:** 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.372E+00	1.182E+02	0	B001	2 0 1 0 0	
1.122E+00	9.666E+01	10	B001	2 0 1 0 0	
1.021E+00	8.792E+01	15	B001	2 0 1 0 0	
9.351E-01	8.054E+01	20	B001	2 0 1 0 0	
8.620E-01	7.425E+01	25	B001	2 0 1 0 0	

483. $C_5H_{10}O$
Diethyl ketone
3-Pentanone
RN: 96-22-0 **MP** (°C)**:** –42
MW: 86.13 **BP** (°C)**:** 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-01	6.727E+01	10	G032	1 2 1 1 2	
4.786E-01	4.123E+01	20	D052	1 1 0 0 1	
5.613E-01	4.834E+01	20	G030	1 2 0 0 2	
6.052E-01	5.213E+01	25	B019	1 0 1 2 0	
3.818E-01	3.288E+01	25	B060	2 0 1 1 1	
5.328E-01	4.589E+01	25	G030	1 2 0 0 2	
5.900E-01	5.082E+01	25	K012	1 0 0 0 1	
4.999E-01	4.306E+01	30	G030	1 2 0 0 1	
5.760E-01	4.961E+01	30	G032	1 2 1 1 2	
4.560E-01	3.928E+01	50	G032	1 2 1 1 2	

484. $C_5H_{10}O$
1-Penten-3-ol
Penten-1-ol-3
RN: 616-25-1 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.312E-01	8.021E+01	20	G031	1 0 0 0 2	
8.798E-01	7.579E+01	25	G031	1 0 0 0 2	
8.340E-01	7.184E+01	30	G031	1 0 0 0 2	

485. $C_5H_{10}O$
4-Penten-1-ol
Penten-4-ol-1
RN: 821-09-0 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 135.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.458E-01	5.562E+01	20	G031	1 0 0 0 2	
6.261E-01	5.393E+01	25	G031	1 0 0 0 2	
6.115E-01	5.267E+01	30	G031	1 0 0 0 2	

486. $C_5H_{10}O$
3-Penten-2-ol
Penten-3-ol-2
RN: 1569-50-2 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	8.642E+01	20	G031	1 0 0 0 2	
9.508E-01	8.189E+01	25	G031	1 0 0 0 2	
9.075E-01	7.817E+01	30	G031	1 0 0 0 2	

487. $C_5H_{10}O$
2-Methyl tetrahydrofuran
2-Methyl oxolane
β-Methyl tetramethylene oxide
RN: 96-47-9 **MP** (°C)**:** –136
MW: 86.13 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E+00	1.011E+02	10	B001	2 0 1 0 0	

488. $C_5H_{10}O$
1-Methyl tetrahydrofuran
Methyl oxolane
α-Methyl tetramethylene oxide
RN: 45376-90-7 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.101E+00	1.810E+02	0	B001	2 0 1 0 0	
1.788E+00	1.540E+02	10	B001	2 0 1 0 0	
1.646E+00	1.418E+02	15	B001	2 0 1 0 0	
1.519E+00	1.308E+02	20	B001	2 0 1 0 0	
1.414E+00	1.218E+02	25	B001	2 0 1 0 0	

489. $C_5H_{10}O$
Cypreth ether
Cyclopropane, ethoxy-
Ethoxycyclopropane
Ethyl cyclopropyl ether
RN: 5614-38-0 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	2.724E+01	25	K061	1 0 1 1 1	
2.500E-01	2.153E+01	25	K061	1 0 1 1 1	

490. $C_5H_{10}O$

3-Methyl-2-butanone
3-Methylbutanone-2

RN: 563-80-4 **MP** (°C)**:** –92
MW: 86.13 **BP** (°C)**:** 94.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.130E-01	7.003E+01	10	G032	1 2 1 1 2	
7.116E-01	6.130E+01	20	G030	1 2 0 0 2	
6.654E-01	5.732E+01	25	G030	1 2 0 0 2	
6.240E-01	5.375E+01	30	G030	1 2 0 0 2	
6.080E-01	5.237E+01	30	G032	1 2 1 1 2	
5.940E-01	5.116E+01	50	G032	1 2 1 1 2	

491. $C_5H_{10}OS_2$

Butylxanthogenic acid

RN: **MP** (°C)**:**
MW: 150.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	1.202E-01	25	K012	1 0 0 0 0	

492. $C_5H_{10}O_2$

Valeric acid
Valeric acid, normal
n-Valeric acid

RN: 109-52-4 **MP** (°C)**:** –34.5
MW: 102.13 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.295E-01	2.344E+01	25	B060	2 0 1 1 1	
4.636E-01	4.735E+01	25	H028	2 0 2 0 2	
3.697E-01	3.776E+01	25	H122	1 0 0 0 2	
4.055E-01	4.141E+01	25	H338	2 2 1 2 2	
3.750E-01	3.830E+01	25	K012	1 0 0 0 2	
4.893E-01	4.997E+01	35	H338	2 2 1 2 2	
2.936E-03	2.999E-01	c	L055	0 0 0 0 1	
4.636E-01	4.735E+01	ns	A406	0 0 0 0 1	

493. $C_5H_{10}O_2$
Methyl butyrate
Buttersaeure-methyl ester
n-Methyl *n*-butyrate
RN: 623-42-7 **MP** (°C)**:** –95
MW: 102.13 **BP** (°C)**:** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-01	1.561E+01	21	F001	1 0 1 2 2	
1.506E-01	1.538E+01	21	F300	1 0 0 0 2	
1.600E-01	1.634E+01	21	S006	1 0 0 0 2	
1.469E-01	1.500E+01	25	A049	1 0 0 0 2	

494. $C_5H_{10}O_2$
3-Hydroxy-2-methyltetrahydrofuran
3-Furanol, tetrahydro-2-methyl-
RN: 29848-44-0 **MP** (°C)**:**
MW: 102.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E+00	1.667E+02	rt	B066	0 2 0 0 1	
4.896E+00	5.000E+02	rt	B066	0 2 0 0 2	

495. $C_5H_{10}O_2$
Propyl acetate
Essigsaeurepropyl ester
RN: 109-60-4 **MP** (°C)**:** –92
MW: 102.13 **BP** (°C)**:** 101.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-01	2.270E+01	20	E002	1 0 0 0 2	
1.850E-01	1.889E+01	20	F001	1 0 1 0 2	
1.821E-01	1.860E+01	20	F300	1 0 0 0 2	
1.800E-01	1.838E+01	20	M171	1 0 0 0 1	
2.220E-01	2.267E+01	21	S006	1 0 0 0 2	
1.920E-01	1.961E+01	25	B060	2 0 1 1 1	
1.731E-01	1.768E+01	30	R318	1 2 0 1 1	
1.960E-01	2.002E+01	37	E028	1 0 1 1 2	

496. $C_5H_{10}O_2$
Pivalic acid
Trimethylacetic acid
Trimethylessigsaeure
RN: 75-98-9 **MP** (°C)**:** 35.5
MW: 102.13 **BP** (°C)**:** 163.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-01	2.170E+01	20	F300	1 0 0 0 2	

497. $C_5H_{10}O_2$
Isopropyl acetate
Essigsaeureisopropyl ester
Iso-propylacetat
RN: 108-21-4 **MP** (°C)**:** –73
MW: 102.13 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-01	2.610E+01	20	D052	1 1 0 0 2	average of 2
3.030E-01	3.095E+01	20	F001	1 0 1 2 2	
2.937E-01	3.000E+01	20	F300	1 0 0 0 2	
2.108E-01	2.153E+01	24.6	H121	2 0 0 0 1	
2.759E-01	2.818E+01	25	B060	2 0 1 1 1	
1.930E-01	1.971E+01	37	E028	1 0 1 1 2	

498. $C_5H_{10}O_2$
Butyl formate
Formic acid butyl ester
RN: 592-84-7 **MP** (°C)**:**
MW: 102.13 **BP** (°C)**:** 106.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-02	1.001E+01	22	S006	1 0 0 0 1	
6.400E-02	6.537E+00	25	K012	1 0 0 0 1	
7.400E-02	7.558E+00	27	B052	1 0 1 1 2	
7.500E-02	7.660E+00	30.5	N014	0 0 0 0 0	
8.100E-02	8.273E+00	40.0	N014	0 0 0 0 0	

499. $C_5H_{10}O_2$
Ethyl propionate
Propanoic acid ethyl ester
RN: 105-37-3 **MP** (°C)**:** –73
MW: 102.13 **BP** (°C)**:** 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.844E-01	1.884E+01	20	D052	1 1 0 0 2	
2.200E-01	2.247E+01	20	S006	1 0 0 0 1	
2.154E-01	2.200E+01	25	F300	1 0 0 0 1	
1.700E-01	1.736E+01	25	K012	1 0 0 0 1	
2.108E-01	2.153E+01	30	R318	1 1 0 1 1	

500. $C_5H_{10}O_2$
Isovaleric acid
Isovaleriansaeure
RN: 503-74-2 **MP** (°C)**:** –29.3
MW: 102.13 **BP** (°C)**:** 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.946E-01	4.031E+01	20	D041	1 0 0 0 1	
3.985E-01	4.070E+01	20	F300	1 0 0 0 2	

501. $C_5H_{10}O_3$
Methyl β-methoxypropionate
Propionic acid, 3-methoxy-, methyl ester
Methyl 3-methoxypropanoate
Methyl 3-methoxypropionate
RN: 3852-09-3 **MP** (°C)**:**
MW: 118.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E+00	4.286E+02	25	R034	1 0 0 0 1	

502. $C_5H_{10}O_3$
Ethyl carbonate
Diethyl carbonate
RN: 105-58-8 **MP** (°C)**:** –43
MW: 118.13 **BP** (°C)**:** 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-01	1.845E+01	20	D052	1 1 0 0 2	

503. $C_5H_{10}O_5$
D-Xylose
α-Xylose
Wood sugar
RN: 58-86-6 **MP** (°C)**:** 144.5
MW: 150.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E+00	4.322E+02	25	G317	0 0 0 0 0	

504. $C_5H_{10}O_5$
L-Arabinose
L-Arabinopyranose
RN: 87-72-9 **MP** (°C)**:** 158
MW: 150.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E+00	3.726E+02	10	F300	1 0 0 0 2	

505. $C_5H_{11}Br$
n-Amyl bromide
1-Bromopentane
Pentyl bromide
Amylene bromide
RN: 110-53-2 **MP** (°C)**:** –87.9
MW: 151.05 **BP** (°C)**:** 129.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.380E-04	1.266E-01	25	M342	1 0 1 1 2	
1.800E-02	2.719E+00	ns	H307	0 0 0 0 0	

506. $C_5H_{11}Br$
Isoamyl bromide
1-Bromo-3-methylbutane
RN: 107-82-4 **MP** (°C)**:** –112
MW: 151.05 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.324E-03	2.000E-01	16	F300	1 0 0 0 1	
1.300E-03	1.964E-01	16.5	F001	1 0 1 0 2	

507. $C_5H_{11}NO$
Pentanamide
Valeramide
RN: 626-97-1 **MP** (°C)**:** 102–104
MW: 101.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-01	5.594E+01	6	H059	0 0 0 0 0	
6.360E-01	6.433E+01	16	H059	0 0 0 0 0	
7.880E-01	7.971E+01	25	H059	0 0 0 0 0	
1.108E+00	1.121E+02	37	H059	0 0 0 0 0	

508. $C_5H_{11}NO_2$
DL-Valine
DL-Valin
RN: 516-06-3 **MP** (°C)**:** 296
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-01	6.552E+01	0	D018	2 2 2 1 2	
5.711E-01	6.690E+01	25	C018	0 0 0 0 0	
6.035E-01	7.070E+01	25	D016	1 0 0 0 2	
5.912E-01	6.926E+01	25	D018	2 2 2 1 2	
5.614E-01	6.577E+01	25	D041	1 0 0 0 2	
5.975E-01	7.000E+01	25	F300	1 0 0 0 0	
7.352E-01	8.612E+01	50	D018	2 2 2 1 2	
7.170E-01	8.400E+01	50	F300	1 0 0 0 1	
1.003E+00	1.175E+02	75	D018	2 2 2 1 2	
9.559E-01	1.120E+02	75	D041	1 0 0 0 2	
9.560E-01	1.120E+02	75	F300	1 0 0 0 2	
1.349E+00	1.580E+02	100	F300	1 0 0 0 2	
1.351E+00	1.583E+02	99.99	P349	0 0 0 0 0	

509. $C_5H_{11}NO_2$
L-Norvaline
L-(+)-2-Aminovaleric acid
RN: 6600-40-4 **MP** (°C)**:** >300
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.286E-01	9.707E+01	15	D041	1 0 0 0 2	

510. $C_5H_{11}NO_2$
tert-Butyl carbamate
O-t-Butyl carbamate
RN: 4248-19-5 **MP** (°C)**:** 105
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.250E+00	1.464E+02	37	H006	1 2 2 1 2	
1.259E+00	1.475E+02	ns	R424	0 0 0 0 0	

511. $C_5H_{11}NO_2$
n-Butyl carbamate
Butyl carbamate
RN: 592-35-8 **MP** (°C)**:** 51
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.577E+01	37	H006	1 2 2 1 1	

512. $C_5H_{11}NO_2$
Isobutyl carbamate
iso-Butyl carbamate
RN: 543-28-2 **MP** (°C)**:** 67
MW: 117.15 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-01	5.857E+01	37	H006	1 2 2 1 0	

513. $C_5H_{11}NO_2$
DL-Isovaline
DL-Isovalin
RN: 595-39-1 **MP** (°C)**:** 315
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E+00	2.809E+02	20	F300	1 0 0 0 2	

514. $C_5H_{11}NO_2$

D-Valine
β-Amino-isovalerian-saeure
β-Aminoisovaleric acid

RN: 640-68-6 **MP** (°C)**:** >295
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-02	1.512E+00	10	D038	1 0 1 0 0	EFG, unit assumed, *sic*
4.296E-01	5.033E+01	20	D041	1 0 0 0 1	
7.053E-01	8.263E+01	25	C018	0 0 0 0 0	
1.343E-02	1.574E+00	25	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.384E-02	1.622E+00	33	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.426E-02	1.671E+00	40	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.455E-02	1.705E+00	49	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.500E-02	1.757E+00	57	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.592E-02	1.865E+00	65	D038	1 0 1 0 0	EFG, unit assumed, *sic*

515. $C_5H_{11}NO_2$

Betaine
Betain

RN: 107-43-7 **MP** (°C)**:** 296
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E+00	6.110E+02	19.30	F300	1 0 0 0 2	

516. $C_5H_{11}NO_2$

DL-Norvaline
DL-2-Aminovaleric acid

RN: 760-78-1 **MP** (°C)**:** 303.0
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.251E-01	9.666E+01	15	D041	1 0 0 0 2	
7.768E-01	9.100E+01	18	F300	1 0 0 0 1	
6.616E-01	7.751E+01	25	K031	2 1 2 1 2	

517. $C_5H_{11}NO_2$

L-Valine
Valine
L-(+)-valine
L-2-Amino-3-methylbutyric acid
2-Amino-3-methylbutyric acid

RN: 72-18-4 **MP** (°C)**:** 315
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.180E-01	8.411E+01	15	D349	2 1 1 2 2	
4.866E-01	5.701E+01	20	B032	1 2 2 1 2	
7.360E-01	8.622E+01	20	D349	2 1 1 2 2	
4.992E-01	5.848E+01	25	B032	1 2 2 1 2	
6.940E-01	8.130E+01	25	D041	1 0 0 0 2	
7.550E-01	8.845E+01	25	D349	2 1 1 2 2	
4.710E-01	5.518E+01	25	G092	2 1 1 1 1	
4.710E-01	5.518E+01	25	G315	0 0 0 0 0	
5.900E-01	6.912E+01	25	N001	0 0 0 0 0	EFG
4.740E-01	5.553E+01	25	N012	2 0 2 1 2	
5.019E-01	5.880E+01	27	D036	0 0 0 0 0	
5.114E-01	5.991E+01	29.80	B032	1 2 2 1 2	
7.929E-01	9.289E+01	65	D041	1 0 0 0 2	

518. $C_5H_{11}NO_2$

3-Nitropentane
Pentane, 3-nitro-

RN: 551-88-2 **MP** (°C)**:**
MW: 117.15 **BP** (°C)**:** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.300E+00	25	A049	1 0 0 0 1	

519. $C_5H_{11}NO_2S$

DL-Methionine
DL-Methionin
DL-2-Amino-4-(methylthio)butyric acid
Acimetion

RN: 59-51-8 **MP** (°C)**:** 281
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	1.790E+01	0	F300	1 0 0 0 2	
1.905E-01	2.843E+01	19.99	F419	0 0 0 0 0	pH 5.81
2.191E-01	3.269E+01	25	D041	1 0 0 0 2	
2.191E-01	3.270E+01	25	F300	1 0 0 0 2	
3.039E-01	4.535E+01	39.99	F419	0 0 0 0 0	pH 5.56

(*continued*)

519. $C_5H_{11}NO_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.211E-01	4.791E+01	44.99	F419	0 0 0 0 0	pH 5.51
3.833E-01	5.720E+01	50	F300	1 0 0 0 2	
4.241E-01	6.328E+01	54.99	F419	0 0 0 0 0	pH 5.39
5.596E-01	8.350E+01	69.99	F419	0 0 0 0 0	pH 5.24
6.379E-01	9.519E+01	75	D041	1 0 0 0 2	
6.380E-01	9.520E+01	75	F300	1 0 0 0 2	
6.965E-01	1.039E+02	79.99	F419	0 0 0 0 0	pH 5.15
1.003E+00	1.497E+02	100	F300	1 0 0 0 2	
2.212E-01	3.300E+01	ns	K444	0 0 0 0 0	

520. $C_5H_{11}NO_2S$

Methionine
L-(–)-Methionine
2-Amino-4-(methylthio)butanoic acid
RN: 63-68-3 **MP** (°C)**:** –279
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.504E-01	5.228E+01	20	B032	1 2 2 1 2	
3.791E-01	5.656E+01	25	B032	1 2 2 1 2	
3.566E-01	5.321E+01	25	G315	0 0 0 0 0	
3.753E-01	5.600E+01	25.1	N024	0 0 0 0 0	
3.746E-01	5.590E+01	25.1	N026	0 0 0 0 0	
3.548E-01	5.294E+01	25.1	N027	1 1 2 2 2	
3.498E-01	5.220E+01	27	D036	0 0 0 0 0	
4.093E-01	6.107E+01	29.80	B032	1 2 2 1 2	

521. $C_5H_{11}NO_2S$

Penicillamine
3,3-Dimethyl-D-(–)-cysteine
D-3-Mercaptovaline
D-Penicillamine
RN: 52-67-5 **MP** (°C)**:** 198.0
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.702E-01	1.000E+02	20	C120	0 0 0 0 0	

522. $C_5H_{11}NO_2.H_2O$

Betaine (monohydrate)
Trimethylammonioacetate (monohydrate)
RN: 590-47-6 **MP** (°C)**:**
MW: 135.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E+00	6.109E+02	19	D041	1 0 0 0 2	

523. C_5H_{12}

Pentane
n-Pentane
RN: 109-66-0 **MP** (°C)**:** –130
MW: 72.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.106E-04	6.570E-02	0	P003	2 2 2 2 2	
5.666E-04	4.088E-02	4.0	N004	1 1 2 2 2	
1.516E-04	1.094E-02	4.8	L007	2 1 1 2 2	
1.516E-04	1.094E-02	5.1	L007	2 0 1 1 2	
5.944E-04	4.289E-02	10.0	N004	1 1 2 2 2	
1.635E-04	1.180E-02	14.8	L007	2 1 1 2 2	
2.425E-04	1.750E-02	20	M337	2 1 2 2 2	
5.444E-04	3.928E-02	20.0	N004	1 1 2 2 2	
1.563E-04	1.128E-02	24.8	L007	2 1 1 2 2	
5.267E-04	3.800E-02	25	A049	1 0 0 0 1	
5.475E-04	3.950E-02	25	K119	1 0 0 0 2	
5.336E-04	3.850E-02	25	M001	2 1 2 2 2	
5.336E-04	3.850E-02	25	M002	2 1 2 2 2	
5.650E-04	4.077E-02	25	M342	1 0 1 1 2	
6.597E-04	4.760E-02	25	P003	2 2 2 2 2	
5.611E-04	4.048E-02	25.0	N004	1 1 2 2 2	
5.475E-04	3.950E-02	25.0	P051	2 1 1 2 2	
5.475E-04	3.950E-02	25.00	P007	2 1 2 2 2	
5.611E-04	4.048E-02	30.0	N004	1 1 2 2 2	
1.509E-04	1.089E-02	34.8	L007	2 1 1 2 2	
5.516E-04	3.980E-02	40.1	P051	2 1 1 2 2	
5.516E-04	3.980E-02	40.10	P007	2 1 2 2 2	
5.793E-04	4.180E-02	55.7	P051	2 1 1 2 2	
5.793E-04	4.180E-02	55.70	P007	2 1 2 2 2	
9.619E-04	6.940E-02	99.1	P051	2 1 1 2 2	
9.619E-04	6.940E-02	99.10	P007	2 1 2 2 2	
1.525E-03	1.100E-01	121.3	P051	2 1 1 2 2	
1.525E-03	1.100E-01	121.30	P007	2 1 2 2 2	
2.786E-03	2.010E-01	137.3	P051	2 1 1 2 2	
2.786E-03	2.010E-01	137.30	P007	2 1 2 2 2	
4.130E-03	2.980E-01	149.5	P051	2 1 1 2 2	
4.130E-03	2.980E-01	149.50	P007	2 1 2 2 2	
1.010E-04	7.287E-03	ns	D348	0 0 0 0 0	

524. C_5H_{12}
2-Methylbutane
Isopentane
Izopentan
RN: 78-78-4 **MP** (°C)**:** –160
MW: 72.15 **BP** (°C)**:** 30

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	7.240E-02	0	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	K119	1 0 0 0 2	
6.625E-04	4.780E-02	25	M001	2 1 2 2 2	
6.625E-04	4.780E-02	25	M002	2 1 2 2 2	
6.874E-04	4.960E-02	25	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	P007	2 1 2 2 2	
6.653E-04	4.800E-02	25	P051	2 1 1 2 2	

525. C_5H_{12}
Neopentane
2,2-Dimethylpropane
RN: 463-82-1 **MP** (°C)**:**
MW: 72.15 **BP** (°C)**:** 9.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-04	1.602E-02	25	D346	0 0 0 0 0	
4.601E-04	3.320E-02	25	M001	2 1 2 2 2	
5.611E-04	4.048E-02	25	S212	2 1 2 2 2	
3.833E-04	2.766E-02	40	S212	2 1 2 2 1	
2.667E-04	1.924E-02	60	S212	2 1 2 2 1	
2.389E-04	1.724E-02	80	S212	2 1 2 2 1	

526. $C_5H_{12}ClO_2PS_2$
Chlormephos
Dotan
Diethyl *S*-(chloromethyl) dithiophosphate
RN: 24934-91-6 **MP** (°C)**:**
MW: 234.70 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-04	6.000E-02	20	L303	1 0 0 0 1	
2.556E-04	6.000E-02	20	M161	1 0 0 0 1	
2.559E-04	6.005E-02	ns	S460	0 0 0 0 0	

527. $C_5H_{12}NO_3PS_2$
Dimethoate
O,O-Dimethyl *S*-(*N*-methylcarbamoylmethyl) dithiophosphate
RN: 60-51-5 **MP** (°C)**:** 52.25
MW: 229.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	2.514E+01	20	B179	0 0 0 0 0	
1.309E-01	3.000E+01	20	G319	0 0 0 0 0	
1.090E-01	2.500E+01	21	M161	1 0 0 0 1	
1.701E-01	3.900E+01	ns	M061	0 0 0 0 1	

528. $C_5H_{12}N_2$
2-Methylpiperazine
2-Methyl-piperazin
RN: 109-07-9 **MP** (°C)**:** 66
MW: 100.16 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.343E+00	4.350E+02	20	F300	1 0 0 0 2	

529. $C_5H_{12}N_2O$
Methyl-*n*-butylnitrosamine
MBN
RN: 7068-83-9 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-01	2.323E+01	24	M031	1 1 1 1 1	

530. $C_5H_{12}O$
2-Methyl-1-butanol
DL-2-Methyl-1-butanol
2-Methylbutan-1-ol
RN: 137-32-6 **MP** (°C)**:** –70
MW: 88.15 **BP** (°C)**:** 128.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.269E-01	3.763E+01	.5	S307	1 1 0 2 2	
3.720E-01	3.279E+01	9.7	S307	1 1 0 2 2	
3.122E-01	2.752E+01	19.6	S307	1 1 0 2 2	
3.496E-01	3.082E+01	20	G004	2 2 2 2 2	
3.304E-01	2.913E+01	25	C093	2 1 1 1 1	
3.272E-01	2.884E+01	25	G004	2 2 2 2 2	
2.778E-01	2.449E+01	29.6	S307	1 1 0 2 2	
3.122E-01	2.752E+01	30	G004	2 2 2 2 2	

(*continued*)

530. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.616E-01	2.306E+01	39.3	S307	1 1 0 2 2	
2.453E-01	2.162E+01	49.6	S307	1 1 0 2 2	
2.301E-01	2.028E+01	59.3	S307	1 1 0 2 2	
2.485E-01	2.191E+01	69.5	S307	1 1 0 2 2	
2.551E-01	2.248E+01	79.7	S307	1 1 0 2 2	
2.724E-01	2.401E+01	90.8	S307	1 1 0 2 2	

531. $C_5H_{12}O$

tert-Isoamyl alcohol
3-Methyl-1-butanol
Isopentyl alcohol
Isoamyl alcohol

RN: 123-51-3 **MP** (°C)**:** –117
MW: 88.15 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.079E-01	3.596E+01	0	S307	1 1 0 2 2	
3.090E-01	2.724E+01	10	A328	0 0 0 0 0	
3.454E-01	3.044E+01	10.1	S307	1 1 0 2 2	
3.347E-01	2.950E+01	15	K002	1 2 1 1 2	
3.130E-01	2.759E+01	18	F001	1 0 1 2 2	
2.918E-01	2.572E+01	19.8	S307	1 1 0 2 2	
3.120E-01	2.750E+01	20	F300	1 0 0 0 2	
3.144E-01	2.771E+01	20	G004	2 2 2 2 2	
3.111E-01	2.743E+01	20	K002	1 2 1 1 2	
9.586E-01	8.450E+01	20	K085	1 0 0 0 2	
2.659E-01	2.344E+01	25	A328	0 0 0 0 0	
3.411E-01	3.007E+01	25	C068	2 2 2 1 2	
2.982E-01	2.629E+01	25	C093	2 1 1 1 1	
3.251E-01	2.865E+01	25	F317	2 1 1 1 2	
2.950E-01	2.601E+01	25	G004	2 2 2 2 2	
2.950E-01	2.601E+01	25	K002	1 2 1 1 2	
2.799E-01	2.468E+01	30	G004	2 2 2 2 2	
2.832E-01	2.496E+01	30	K002	1 2 1 1 2	
2.842E-01	2.506E+01	30.1	H043	2 2 2 2 2	average of 3
2.540E-01	2.239E+01	30.2	S307	1 1 0 2 2	
2.442E-01	2.153E+01	40	A328	0 0 0 0 0	
2.420E-01	2.133E+01	40.0	S307	1 1 0 2 2	
2.257E-01	1.990E+01	49.9	S307	1 1 0 2 2	
2.431E-01	2.143E+01	59.8	S307	1 1 0 2 2	
2.344E-01	2.066E+01	70.0	S307	1 1 0 2 2	
2.442E-01	2.153E+01	80.0	S307	1 1 0 2 2	
2.518E-01	2.220E+01	90.0	S307	1 1 0 2 2	
2.836E-01	2.500E+01	ns	L003	0 0 2 1 2	
2.767E-01	2.439E+01	rt	H111	0 0 0 0 1	

532. $C_5H_{12}O$
Neopentyl alcohol
t-Butyl carbinol
RN: 75-84-3 **MP** (°C)**:** 53
MW: 88.15 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.048E-01	3.568E+01	12.0	S307	1 1 0 2 2	
3.826E-01	3.372E+01	18.8	S307	1 1 0 2 2	
4.090E-01	3.605E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	G004	2 2 2 2 2	
3.603E-01	3.176E+01	30	G004	2 2 2 2 2	
3.229E-01	2.847E+01	30.0	S307	1 1 0 2 2	
2.982E-01	2.629E+01	40.0	S307	1 1 0 2 2	
2.616E-01	2.306E+01	50.0	S307	1 1 0 2 2	
2.778E-01	2.449E+01	60.0	S307	1 1 0 2 2	
2.399E-01	2.114E+01	70.2	S307	1 1 0 2 2	
2.864E-01	2.525E+01	80.0	S307	1 1 0 2 2	
2.637E-01	2.325E+01	90.0	S307	1 1 0 2 2	

533. $C_5H_{12}O$
Methyl *tert*-butyl ether
tert-Butyl methyl ether
RN: 1634-04-4 **MP** (°C)**:** –109
MW: 88.15 **BP** (°C)**:** 54.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.564E-01	5.786E+01	2.34	S461	0 0 0 0 0	
6.236E-01	5.497E+01	9.99	S461	0 0 0 0 0	
5.196E-01	4.580E+01	20	E019	1 0 1 1 1	
4.738E-01	4.177E+01	24.99	S461	0 0 0 0 0	
5.815E-01	5.126E+01	25	K072	1 0 1 1 1	
5.815E-01	5.126E+01	25	M087	1 1 2 1 2	

534. $C_5H_{12}O$
3-Pentanol
Pentan-3-ol
Diethyl carbinol
RN: 584-02-1 **MP** (°C)**:** <25
MW: 88.15 **BP** (°C)**:** 115.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.704E-01	7.672E+01	0	S307	1 1 0 2 2	
7.382E-01	6.507E+01	10.2	S307	1 1 0 2 2	
6.026E-01	5.312E+01	20	G004	2 2 2 2 2	

(*continued*)

534. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-01	5.536E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	25	C093	2 1 1 1 1	
5.556E-01	4.898E+01	25	G004	2 2 2 2 2	
5.144E-01	4.535E+01	30	G004	2 2 2 2 2	
5.730E-01	5.051E+01	30.0	S307	1 1 0 2 2	
4.510E-01	3.975E+01	40.0	S307	1 1 0 2 2	
4.604E-01	4.058E+01	50.0	S307	1 1 0 2 2	
3.889E-01	3.428E+01	60.0	S307	1 1 0 2 2	
3.783E-01	3.335E+01	70.0	S307	1 1 0 2 2	
3.635E-01	3.204E+01	80.0	S307	1 1 0 2 2	
3.773E-01	3.326E+01	90.0	S307	1 1 0 2 2	
1.392E+00	1.227E+02	ns	L003	0 0 2 1 1	
5.196E-01	4.580E+01	rt	H111	0 0 0 0 1	

535. $C_5H_{12}O$

3-Methyl-2-butanol
Methylisopropylcarbinol

RN: 598-75-4 **MP** (°C)**:** <25
MW: 88.15 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.771E-01	7.732E+01	0	S307	1 1 0 2 2	
7.609E-01	6.708E+01	10.1	S307	1 1 0 2 2	
6.492E-01	5.723E+01	20	G004	2 2 2 2 2	
6.381E-01	5.625E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	30	G004	2 2 2 2 2	
5.536E-01	4.880E+01	30.0	S307	1 1 0 2 2	
4.833E-01	4.260E+01	40.0	S307	1 1 0 2 2	
4.416E-01	3.892E+01	50.0	S307	1 1 0 2 2	
3.720E-01	3.279E+01	60.0	S307	1 1 0 2 2	
4.005E-01	3.531E+01	70.0	S307	1 1 0 2 2	
3.942E-01	3.475E+01	79.5	S307	1 1 0 2 2	
3.942E-01	3.475E+01	90.0	S307	1 1 0 2 2	

536. $C_5H_{12}O$

Ethylisopropyl ether
Propane, 2-ethoxy-

RN: 625-54-7 **MP** (°C)**:**
MW: 88.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.409E+01	ns	J300	0 0 0 0 0	

537. $C_5H_{12}O$

1-Pentanol
Amyl alcohol
Pentanol
Pentyl alcohol
n-Amyl alcohol

RN: 71-41-0 **MP** (°C)**:** –79
MW: 88.15 **BP** (°C)**:** 138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.321E-01	3.809E+01	–.5	F051	2 1 0 1 2	
3.358E-01	2.960E+01	0	E029	1 2 0 1 2	
3.635E-01	3.204E+01	0	S307	1 1 0 2 2	
3.709E-01	3.269E+01	7	F051	2 1 0 1 2	
2.982E-01	2.629E+01	10	E029	1 2 0 1 2	
2.864E-01	2.525E+01	10.2	S307	1 1 0 2 2	
3.068E-01	2.705E+01	14	F051	2 1 0 1 2	
3.004E-01	2.648E+01	15	F051	2 1 0 1 2	
5.395E+00	4.756E+02	15.5	F051	2 1 0 1 2	
2.875E-01	2.534E+01	16.5	F051	2 1 0 1 2	
2.821E-01	2.487E+01	18	F051	2 1 0 1 2	
2.453E-01	2.162E+01	20	A015	1 2 1 1 2	
1.020E-02	8.992E-01	20	D052	1 1 0 0 0	*sic*
2.605E-01	2.296E+01	20	E029	1 2 0 1 2	
2.616E-01	2.306E+01	20	G004	2 2 2 2 2	
1.676E-01	1.478E+01	20	L049	1 1 2 1 1	
3.070E-01	2.706E+01	20	M312	1 0 0 0 1	
2.496E-01	2.200E+01	20.2	S307	1 1 0 2 2	
3.607E-01	3.180E+01	22	H072	1 0 1 1 2	
2.691E-01	2.372E+01	23	F051	2 1 0 1 2	
3.730E-01	3.288E+01	25	B019	1 0 1 2 0	
2.451E-01	2.160E+01	25	B038	1 0 1 1 2	
1.896E-01	1.672E+01	25	B060	2 0 1 1 1	
2.442E-01	2.153E+01	25	C093	2 1 1 1 1	
1.000E+00	8.815E+01	25	F044	1 0 0 0 0	EFG
2.137E-01	1.884E+01	25	F317	2 1 1 1 2	
2.431E-01	2.143E+01	25	G004	2 2 2 2 2	
2.300E-01	2.027E+01	25	G075	1 0 1 0 1	
2.810E-01	2.477E+01	25	H028	2 0 2 0 2	
2.817E-01	2.483E+01	25	H104	1 0 0 0 1	
2.500E-01	2.204E+01	25	K025	2 2 1 1 1	
2.561E-01	2.258E+01	29	F051	2 1 0 1 2	
2.333E-01	2.057E+01	30	E029	1 2 0 1 2	
2.257E-01	1.990E+01	30	G004	2 2 2 2 2	
2.246E-01	1.980E+01	30.6	S307	1 1 0 2 2	
5.368E+00	4.732E+02	34.0	F051	2 1 0 1 2	
2.475E-01	2.181E+01	36	F051	2 1 0 1 2	
2.130E-01	1.878E+01	37	E028	1 0 1 1 2	
2.115E-01	1.865E+01	40	E029	1 2 0 1 2	
2.082E-01	1.836E+01	40.2	S307	1 1 0 2 2	
2.006E-01	1.768E+01	50	E029	1 2 0 1 2	

(*continued*)

537. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-01	1.797E+01	50.0	S307	1 1 0 2 2	
2.475E-01	2.181E+01	58	F051	2 1 0 1 2	
2.006E-01	1.768E+01	60	E029	1 2 0 1 2	
2.039E-01	1.797E+01	60.3	S307	1 1 0 2 2	
5.290E+00	4.664E+02	69.5	F051	2 1 0 1 2	
2.061E-01	1.816E+01	70	E029	1 2 0 1 2	
2.170E-01	1.913E+01	70.0	S307	1 1 0 2 2	
2.561E-01	2.258E+01	72.0	F051	2 1 0 1 2	
2.115E-01	1.865E+01	80	E029	1 2 0 1 2	
2.213E-01	1.951E+01	80.0	S307	1 1 0 2 2	
2.691E-01	2.372E+01	81	F051	2 1 0 1 2	
2.821E-01	2.487E+01	87	F051	2 1 0 1 2	
2.224E-01	1.961E+01	90	E029	1 2 0 1 2	
2.453E-01	2.162E+01	90.7	S307	1 1 0 2 2	
2.875E-01	2.534E+01	91	F051	2 1 0 1 2	
3.004E-01	2.648E+01	95	F051	2 1 0 1 2	
5.180E+00	4.566E+02	97.3	F051	2 1 0 1 2	
3.068E-01	2.705E+01	98	F051	2 1 0 1 2	
2.496E-01	2.200E+01	100	E029	1 2 0 1 2	
2.875E-01	2.534E+01	110	E029	1 2 0 1 2	
3.709E-01	3.269E+01	112	F051	2 1 0 1 2	
3.304E-01	2.913E+01	120	E029	1 2 0 1 2	
5.048E+00	4.450E+02	122.3	F051	2 1 0 1 2	
4.321E-01	3.809E+01	126	F051	2 1 0 1 2	
3.889E-01	3.428E+01	130	E029	1 2 0 1 2	
4.677E-01	4.123E+01	140	E029	1 2 0 1 2	
5.351E-01	4.717E+01	140	F051	2 1 0 1 2	
4.896E+00	4.316E+02	141.6	F051	2 1 0 1 2	
5.853E-01	5.159E+01	145	F051	2 1 0 1 2	
6.290E-01	5.545E+01	148.5	F051	2 1 0 1 2	
5.761E-01	5.078E+01	150	E029	1 2 0 1 2	
4.707E+00	4.149E+02	157.3	F051	2 1 0 1 2	
7.322E-01	6.455E+01	160	E029	1 2 0 1 2	
9.060E-01	7.987E+01	167.0	F051	2 1 0 1 2	
9.889E-01	8.717E+01	170	E029	1 2 0 1 2	
1.001E+00	8.826E+01	171.2	F051	2 1 0 1 2	
4.374E+00	3.856E+02	174.0	F051	2 1 0 1 2	
1.690E+00	1.489E+02	180	E029	1 2 0 1 2	
4.089E+00	3.605E+02	181.3	F051	2 1 0 1 2	
1.435E+00	1.265E+02	182.5	F051	2 1 0 1 2	
3.774E+00	3.327E+02	185.2	F051	2 1 0 1 2	
1.833E+00	1.616E+02	186.0	F051	2 1 0 1 2	
2.270E+00	2.001E+02	186.5	F051	2 1 0 1 2	
3.472E+00	3.061E+02	186.5	F051	2 1 0 1 2	
3.237E+00	2.854E+02	187.4	F051	2 1 0 1 2	
3.040E+00	2.680E+02	187.5	F051	2 1 0 1 2	
2.810E-01	2.477E+01	ns	A406	0 0 0 0 1	
2.538E-01	2.237E+01	ns	L003	0 0 2 1 2	
2.224E-01	1.961E+01	rt	H111	0 0 0 0 1	

538. $C_5H_{12}O$

2-Pentanol
iso-Amyl alcohol
sec-Amyl alcohol
Methyl propyl carbinol

RN: 6032-29-7 **MP** (°C)**:** –50
MW: 88.15 **BP** (°C)**:** 119.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.708E-01	6.795E+01	0	S307	1 1 0 2 2	
6.189E-01	5.455E+01	10.1	S307	1 1 0 2 2	
5.030E-01	4.434E+01	19.5	S307	1 1 0 2 2	
4.573E-01	4.031E+01	20	C042	0 0 0 0 0	
1.473E-02	1.298E+00	20	D052	1 1 0 0 0	*sic*
4.538E-01	4.000E+01	20	F300	1 0 0 0 1	
5.258E-01	4.635E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	B019	1 0 1 2 0	
4.843E-01	4.270E+01	25	G004	2 2 2 2 2	
4.499E-01	3.966E+01	30	G004	2 2 2 2 2	
4.300E-01	3.791E+01	30.6	S307	1 1 0 2 2	
3.900E-01	3.438E+01	40.0	S307	1 1 0 2 2	
3.645E-01	3.213E+01	50.0	S307	1 1 0 2 2	
3.432E-01	3.026E+01	60.0	S307	1 1 0 2 2	
3.379E-01	2.979E+01	70.1	S307	1 1 0 2 2	
3.443E-01	3.035E+01	79.9	S307	1 1 0 2 2	
3.368E-01	2.969E+01	90.3	S307	1 1 0 2 2	
5.149E-01	4.539E+01	ns	L003	0 0 2 1 2	

539. $C_5H_{12}O$

tert-Pentyl alcohol
Dimethylethylcarbinol
tert-Amylalkohol

RN: 75-85-4 **MP** (°C)**:**
MW: 88.15 **BP** (°C)**:** 102.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.548E+00	1.364E+02	.5	S307	1 1 0 2 2	
1.462E+00	1.289E+02	9.8	S307	1 1 0 2 2	
1.259E+00	1.110E+02	20	F300	1 0 0 0 2	
1.229E+00	1.083E+02	20	G004	2 2 2 2 2	
1.170E+00	1.031E+02	20.8	S307	1 1 0 2 2	
1.124E+00	9.910E+01	25	G004	2 2 2 2 2	
5.965E-01	5.258E+01	25	G004	2 2 2 2 2	
1.026E+00	9.041E+01	29.5	S307	1 1 0 2 2	
1.041E+00	9.173E+01	30	G004	2 2 2 2 2	
8.549E-01	7.536E+01	39.5	S307	1 1 0 2 2	
7.649E-01	6.743E+01	49.0	S307	1 1 0 2 2	
6.673E-01	5.882E+01	60.0	S307	1 1 0 2 2	
6.391E-01	5.634E+01	70.2	S307	1 1 0 2 2	
6.117E-01	5.393E+01	80.1	S307	1 1 0 2 2	
5.883E-01	5.186E+01	90.2	S307	1 1 0 2 2	
1.124E+00	9.910E+01	rt	H111	0 0 0 0 2	

540. $C_5H_{12}O_2$
Formaldehyde diethyl acetal
Diethoxymethane
Diethylacetalformaldehyde
Formaldehyd-diaethyl-acetal
RN: 462-95-3 **MP** (°C)**:**
MW: 104.15 **BP** (°C)**:** 87.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.721E-01	7.000E+01	18	F300	1 0 0 0 1	

541. $C_5H_{12}O_4$
Pentaerythritol
2,2-bis(Hydroxymethyl)-1,3-propanediol
PE 200
Tetramethylolmethane
RN: 115-77-5 **MP** (°C)**:** 260
MW: 136.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-01	3.846E+01	0	M043	1 0 0 0 0	
3.498E-01	4.762E+01	10	M043	1 0 0 0 0	
3.863E-01	5.260E+01	15	F300	1 0 0 0 2	
4.157E-01	5.660E+01	20	M043	1 0 0 0 0	
5.441E-01	7.407E+01	30	M043	1 0 0 0 0	
8.450E-01	1.150E+02	40	M043	1 0 0 0 1	
1.324E+00	1.803E+02	60	M043	1 0 0 0 1	
2.099E+00	2.857E+02	80	M043	1 0 0 0 1	
3.672E+00	5.000E+02	100	M043	1 0 0 0 2	
3.890E-01	5.297E+01	ns	R424	0 0 0 0 0	

542. $C_5H_{12}O_5$
Adonitol
Adonit
Adonite
RN: 488-81-3 **MP** (°C)**:** 104
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E+00	6.016E+02	25	C346	0 0 0 0 0	

543. $C_5H_{12}O_5$
Xylitol
RN: 87-99-0 **MP** (°C)**:** 96 K
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.798E+00	5.778E+02	20.12	W414	0 0 0 0 0	
3.963E+00	6.030E+02	25.1	W414	0 0 0 0 0	
4.153E+00	6.319E+02	30.01	W414	0 0 0 0 0	
4.355E+00	6.627E+02	35.05	W414	0 0 0 0 0	
4.550E+00	6.922E+02	40.13	W414	0 0 0 0 0	
4.721E+00	7.183E+02	45.10	W414	0 0 0 0 0	
4.873E+00	7.414E+02	50.09	W414	0 0 0 0 0	
5.001E+00	7.610E+02	55.05	W414	0 0 0 0 0	

544. $C_5H_{12}O_5$
DL-Arabinitol
(±)-Arabitol
RN: 2152-56-9 **MP** (°C)**:** 103
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.459E+00	6.785E+02	25	C346	0 0 0 0 0	

545. $C_5H_{13}N$
N-Methyldiethylamine
N,N-Diethylmethylamine
RN: 616-39-7 **MP** (°C)**:**
MW: 87.17 **BP** (°C)**:** 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E+00	3.105E+02	49.40	C086	2 2 2 2 2	average of 5
4.453E+00	3.881E+02	49.50	C086	2 2 2 2 2	
2.236E+00	1.949E+02	49.80	C086	2 2 2 2 2	
5.715E+00	4.982E+02	50.50	C086	2 2 2 2 2	
1.581E+00	1.378E+02	51.20	C086	2 2 2 2 2	
1.413E+00	1.231E+02	52.00	C086	2 2 2 2 2	
6.981E+00	6.085E+02	53.10	C086	2 2 2 2 2	
7.246E+00	6.316E+02	54.00	C086	2 2 2 2 2	

546. $C_5H_{13}O_3PS_2$
Demephion
O,O-Dimethyl 2-methylmercaptoethyl thiophosphate
Thiolo-tinox
RN: 8065-62-1 **MP** (°C)**:**
MW: 216.26 **BP** (°C)**:** 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.312E-03	5.000E-01	20	M061	1 0 0 0 2	form II
9.248E-03	2.000E+00	ns	M061	0 0 0 0 2	form I
1.387E-02	3.000E+00	rt	M161	0 0 0 0 0	form II
1.387E-03	3.000E-01	rt	M161	0 0 0 0 2	form I

547. C_5Cl_6
Hexachlorocyclopentadiene
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene
Hexachloro-1,3-cyclopentadiene
1,2,3,4,5,5-Hexachlorocyclopentadiene
RN: 77-47-4 **MP** (°C)**:** –9.9
MW: 272.77 **BP** (°C)**:** 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-06	8.050E-04	22.5	G301	0 0 0 0 0	

548. $C_6HCl_3N_2S$
4,5,7-Trichloro-2,1,3-benzothiadiazole
PH 40-21
TH 052 H
RN: 1982-55-4 **MP** (°C)**:** 131.5
MW: 239.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.263E-06	1.500E-03	10	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	M061	1 0 0 0 1	
1.795E-05	4.300E-03	30	B200	1 0 0 0 1	

549. $C_6HCl_4NO_2$
2,3,4,5-Tetrachloronitrobenzene
1,2,3,4-Tetrachloro-5-nitrobenzene
2,3,4,5-Tetrachloro-1-nitrobenzene
1-Nitro-2,3,4,5-tetrachlorobenzene
RN: 879-39-0 **MP** (°C)**:** 66.0
MW: 260.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.305E-03	20	E308	1 2 2 1 1	

550. $C_6HCl_4NO_2$
2,3,4,6-Tetrachloronitrobenzene
Benzene, 1,2,3,5-tetrachloro-4-nitro-
RN: 3714-62-3 **MP** (°C)**:**
MW: 260.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-05	7.566E-03	20	E308	1 2 2 1 1	

551. $C_6HCl_4NO_2$
2,3,5,6-Tetrachloronitrobenzene
Tecnazene
RN: 117-18-0 **MP** (°C)**:** 99.5
MW: 260.89 **BP** (°C)**:** 304.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-06	2.087E-03	20	E308	1 2 2 1 0	

552. C_6HCl_5
Pentachlorobenzene
Penta-chlorobenzene
RN: 608-93-5 **MP** (°C)**:** 82
MW: 250.34 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-06	2.503E-04	20	K337	1 0 0 0 2	
9.550E-07	2.391E-04	22	K305	1 0 1 1 0	
1.538E-06	3.850E-04	23	C305	1 1 2 2 2	
5.320E-06	1.332E-03	25	B173	2 0 2 2 2	
2.600E-06	6.509E-04	25	B317	0 0 0 0 0	
3.320E-06	8.311E-04	25	M342	1 0 1 1 2	
3.320E-06	8.311E-04	ns	M308	0 0 1 1 2	

553. C_6HCl_5O
Pentachlorophenol
PCP
2,3,4,5,6-Pentachloro-phenol-
Phenol, 2,3,4,5,6-pentachloro-
Dowicide 7
Fungifen
RN: 87-86-5 **MP** (°C)**:** 174
MW: 266.34 **BP** (°C)**:** 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.877E-05	5.000E-03	0	C310	0 0 0 0 0	
1.877E-05	5.000E-03	0	G310	1 0 0 0 0	
1.877E-05	5.000E-03	0	M061	1 0 0 0 0	

(*continued*)

553. C_6HCl_5O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-05	1.400E-02	20	B185	0 0 0 0 0	
5.256E-05	1.400E-02	22.5	G301	0 0 0 0 0	
6.195E-05	1.650E-02	25	B183	0 0 0 0 1	
8.260E-05	2.200E-02	25	B185	0 0 0 0 0	
3.600E-05	9.588E-03	25	B316	0 0 0 0 0	
6.908E-05	1.840E-02	25	M373	1 0 2 1 2	
5.256E-05	1.400E-02	25	O320	0 0 0 0 0	
8.035E-05	2.140E-02	25.1	A400	2 1 2 2 2	
5.256E-05	1.400E-02	26.70	L095	2 2 1 1 2	
6.758E-05	1.800E-02	27	C310	0 0 0 0 0	
6.758E-05	1.800E-02	27	G310	1 0 0 0 1	
6.758E-05	1.800E-02	27	M061	1 0 0 0 1	
3.484E-03	9.280E-01	30	A400	2 1 2 2 2	
7.509E-05	2.000E-02	30	M161	1 0 0 0 1	
1.126E-04	3.000E-02	50	B200	1 0 0 0 0	
1.314E-04	3.500E-02	50	C310	0 0 0 0 0	
1.314E-04	3.500E-02	50	G310	1 0 0 0 1	
1.314E-04	3.500E-02	50	M061	1 0 0 0 1	
2.178E-04	5.800E-02	62	C310	0 0 0 0 0	
2.178E-04	5.800E-02	62	G310	1 0 0 0 1	
3.191E-04	8.499E-02	70	C310	0 0 0 0 0	
3.191E-04	8.499E-02	70	G310	1 0 0 0 1	
7.509E-05	2.000E-02	ns	L311	0 0 0 0 1	
7.134E-05	1.900E-02	ns	M110	0 0 0 0 0	EFG
6.007E-06	1.600E-03	ns	N013	0 0 0 0 1	

554. C_6HF_5O

Pentafluorophenol

PFP

RN: 771-61-9 **MP** (°C)**:** 34–36

MW: 184.07 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	5.522E+01	25	P031	0 0 0 0 0	

555. $C_6H_2Br_2ClNO_2$

2,6-Dibromoquinone-3-chlorimide

2,6-Dibromoquinonechloroimide

RN: **MP** (°C)**:**

MW: 315.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	6.307E-02	20	G043	1 0 1 1 0	

556. $C_6H_2Br_4$

1,2,4,5-Tetrabromobenzene

RN: 636-28-2 **MP** (°C)**:**
MW: 393.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.724E-08	1.860E-05	10	K440	0 0 0 0 0	
1.105E-07	4.350E-05	25	K440	0 0 0 0 0	
1.976E-07	7.780E-05	35	K440	0 0 0 0 0	

557. $C_6H_2ClN_3O_6$

2,4,6-Trinitro-1-chlorobenzene
Picryl chloride
2-Chlor-1,3,5-trinitrobenzol
Chlorure de picryle

RN: 88-88-0 **MP** (°C)**:**
MW: 247.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.190E-04	1.780E-01	15	D066	1 2 0 0 2	
7.189E-04	1.780E-01	15	D071	1 2 0 0 2	
7.271E-04	1.800E-01	15	F300	1 0 0 0 1	
2.141E-03	5.300E-01	16	D066	1 2 0 0 2	
2.140E-03	5.297E-01	50	D071	1 2 0 0 1	
1.398E-02	3.460E+00	100	D066	1 2 0 0 2	
1.393E-02	3.448E+00	100	D071	1 2 0 0 2	
1.454E-02	3.600E+00	100	F300	1 0 0 0 1	

558. $C_6H_2Cl_2O_4$

Chloranilic acid
Chloranilsaeure

RN: 87-88-7 **MP** (°C)**:** 283
MW: 208.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.091E-03	1.900E+00	14	F300	1 0 0 0 1	
6.699E-02	1.400E+01	99	F300	1 0 0 0 1	

559. $C_6H_2Cl_3NO_2$

2,4,5-Trichloronitrobenzene
1,2,4-Trichloro-5-nitrobenzene
2,4,5-Trichloro-1-nitrobenzene
1,4,5-Trichloro-2-nitrobenzene
3,4,6-Trichloronitrobenzene

RN: 89-69-0 **MP** (°C)**:** 57
MW: 226.45 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.944E-02	20	E308	1 2 2 1 2	

560. $C_6H_2Cl_3NO_2$
2,3,4-Trichloronitrobenzene
1,2,3-Trichloro-4-nitrobenzene
2,3,4-Trichloro-1-nitrobenzene
RN: 17700-09-3 **MP** (°C)**:** 55.5
MW: 226.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.604E-02	20	E308	1 2 2 1 2	

561. $C_6H_2Cl_4$
1,2,4,5-Tetrachlorobenzene
s-Tetrachlorobenzene
RN: 95-94-3 **MP** (°C)**:** 139
MW: 215.89 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.445E-06	3.121E-04	20	K337	1 0 0 0 2	
1.349E-06	2.912E-04	22	K305	1 0 1 1 1	
2.154E-06	4.650E-04	25	B304	2 0 2 2 2	
5.900E-06	1.274E-03	25	B317	0 0 0 0 0	
1.090E-05	2.353E-03	25	M342	1 0 1 1 2	
1.600E-06	3.454E-04	25.2	T428	0 0 0 0 0	
1.806E-06	3.900E-04	ns	B393	0 0 0 0 0	
1.090E-05	2.353E-03	ns	M308	0 0 1 1 2	

562. $C_6H_2Cl_4$
Trichlorobenzyl chloride
TCBC
RN: 1344-32-7 **MP** (°C)**:**
MW: 215.89 **BP** (°C)**:** 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.264E-06	2.000E-03	25	B200	1 0 0 0 0	

563. $C_6H_2Cl_4$
1,2,3,4-Tetrachlorobenzene
Benzene, 1,2,3,4-tetrachloro-
RN: 634-66-2 **MP** (°C)**:** 48
MW: 215.89 **BP** (°C)**:** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-05	3.422E-03	20	K337	1 0 0 0 2	
3.326E-05	7.180E-03	23	C305	1 1 2 2 2	
2.742E-05	5.920E-03	25	B304	2 0 2 2 2	
3.600E-05	7.772E-03	25	B317	0 0 0 0 0	
5.650E-05	1.220E-02	25	M342	1 0 1 1 2	
5.650E-05	1.220E-02	ns	M308	0 0 1 1 2	

564. $C_6H_2Cl_4$

1,2,3,5-Tetrachlorobenzene
1,2,4,6-Tetrachlorobenzene

RN: 634-90-2 **MP** (°C)**:** 50
MW: 215.89 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	2.159E-03	20	K337	1 0 0 0 2	
1.148E-05	2.479E-03	22	K305	1 0 1 1 2	
1.496E-05	3.230E-03	23	C305	1 1 2 2 2	
1.860E-05	4.016E-03	25	B173	2 0 2 2 2	
2.362E-05	5.100E-03	25	B304	2 0 2 2 2	
1.660E-05	3.584E-03	25	B317	0 0 0 0 0	
1.340E-05	2.893E-03	25	M342	1 0 1 1 2	
1.654E-05	3.570E-03	ns	H123	0 0 0 0 0	
1.340E-05	2.893E-03	ns	M308	0 0 1 1 2	

565. $C_6H_2Cl_4O$

2,3,4,6-Tetrachlorophenol
Phenol, 2,3,4,6-tetrachloro-
1-Hydroxy-2,3,4,6-tetrachlorobenzene
TCP

RN: 58-90-2 **MP** (°C)**:**
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.900E-04	1.832E-01	25	B316	0 0 0 0 0	

566. $C_6H_2Cl_4O$

2,3,4,5-Tetrachlorophenol
Phenol, 2,3,4,5-tetrachloro-

RN: 4901-51-3 **MP** (°C)**:** 116
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.158E-04	1.660E-01	25	M373	1 0 2 1 2	

567. $C_6H_2Cl_4O$

2,3,5,6-Tetrachlorophenol
Phenol, 2,3,5,6-tetrachloro-

RN: 935-95-5 **MP** (°C)**:** 115
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.312E-04	1.000E-01	25	M373	1 0 2 1 2	

568. $C_6H_2Cl_4O_2$
Tetrachlorohydroquinone
2,3,5,6-Tetrachlorohydroquinone
RN: 87-87-6 **MP** (°C)**:**
MW: 247.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.673E-05	2.150E-02	ns	L311	0 0 0 0 1	

569. $C_6H_2F_4$
1,2,4,5-Tetrafluorobenzene
2,3,5,6-Tetrafluorobenzene
p-Tetrafluorobenzene
RN: 327-54-8 **MP** (°C)**:** 4.5
MW: 150.08 **BP** (°C)**:** 89.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.215E-03	6.326E-01	25	B349	2 0 2 0 2	

570. $C_6H_2F_4$
1,2,3,5-Tetrafluorobenzene
1,2,4,6-Tetrafluorobenzene
m-Tetrafluorobenzene
1,3,4,5-Tetrafluorobenzene
RN: 2367-82-0 **MP** (°C)**:** –48
MW: 150.08 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-03	7.431E-01	25	B349	2 0 2 0 2	

571. $C_6H_2F_4O$
2,3,5,6-Tetrafluorophenol
1,2,4,5-Tetrafluoro-3-hydroxybenzene
RN: 769-39-1 **MP** (°C)**:** 38
MW: 166.08 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-01	6.145E+01	25	P031	0 0 0 0 0	

572. $C_6H_3Br_2NO_2$
2,6-Dibromoquinone oxime
RN: **MP** (°C)**:**
MW: 280.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-04	2.388E-01	20	G066	1 0 0 0 1	

573. $C_6H_3Br_3$
1,2,4-Tribromobenzene
Tribromobenzene, 1,2,4-
RN: 615-54-3 **MP** (°C)**:** 43
MW: 314.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E-05	3.670E-03	10	K440	0 0 0 0 0	
2.290E-05	7.210E-03	25	K440	0 0 0 0 0	
3.494E-05	1.100E-02	35	K440	0 0 0 0 0	

574. $C_6H_3Br_3O$
2,4,6-Tribromobiphenyl
1,1′-Biphenyl, 2,4,6-tribromo-
RN: 59080-33-0 **MP** (°C)**:** 66
MW: 330.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.111E-02	1.360E+01	26.5	G312	0 0 0 0 0	

575. $C_6H_3Br_3O$
2,4,6-Tribromophenol
2,4,6-Tribrom-phenol
Tribromophenol
Bromol
RN: 118-79-6 **MP** (°C)**:** 95
MW: 330.82 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.116E-04	7.000E-02	15	F300	1 0 0 0 1	
2.300E-04	7.609E-02	ns	O310	0 0 0 0 1	

576. $C_6H_3ClN_2O_4$
1-Chloro-2,4-dinitrobenzene
2,4-Dinitro-1-chlorobenzene
4-Chlor-1,3-dinitrobenzol
4-Chloro-1,3-dinitrobenzene
RN: 97-00-7 **MP** (°C)**:** 53
MW: 202.55 **BP** (°C)**:** 315

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-05	8.000E-03	15	D071	1 2 0 0 0	
3.950E-05	8.000E-03	15	F300	1 0 0 0 0	
4.560E-05	9.236E-03	25	G090	2 2 1 1 1	
2.023E-03	4.098E-01	50	D071	1 2 0 0 1	
7.837E-03	1.587E+00	100	D071	1 2 0 0 2	
8.393E-03	1.700E+00	100	F300	1 0 0 0 1	
7.244E-04	1.467E-01	ns	R427	0 0 0 0 0	

577. $C_6H_3ClN_4$
7-Chloropteridine
Pteridine, 7-chloro-
RN: 1125-84-4 **MP** (°C)**:** 95
MW: 166.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-01	2.174E+01	20	A083	1 2 0 0 0	

578. $C_6H_3Cl_2NO_2$
3,4-Dichloronitrobenzene
1,2-Dichloro-4-nitrobenzene
RN: 99-54-7 **MP** (°C)**:** 41.25
MW: 192.00 **BP** (°C)**:** 255.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.290E-04	1.208E-01	20	E308	1 2 2 1 2	

579. $C_6H_3Cl_2NO_2$
2,5-Dichloronitrobenzene
1,4-Dichloro-2-nitrobenzene
RN: 89-61-2 **MP** (°C)**:** 55.5
MW: 192.00 **BP** (°C)**:** 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	9.216E-02	20	E308	1 2 2 1 2	

580. $C_6H_3Cl_2NO_2$
2,3-Dichloronitrobenzene
1,2-Dichloro-3-nitrobenzene
RN: 3209-22-1 **MP** (°C)**:** 61.5
MW: 192.00 **BP** (°C)**:** 257.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-04	6.240E-02	20	E308	1 2 2 1 2	

581. $C_6H_3Cl_2NO_2$
3,6-Dichloropicolinic acid
3,6-Dichloro-2-pyridinecarboxylic acid
Clopyralid
Lontrel
Stinger
RN: 1702-17-6 **MP** (°C)**:** 151.5
MW: 192.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.208E-03	1.000E+00	20	M161	1 0 0 0 0	
5.208E-03	1.000E+00	ns	K138	0 0 0 0 1	

582. $C_6H_3Cl_3$
1,2,3-Trichlorobenzene
Benzene, 1,2,3-trichloro-
vic-Trichlorobenzene
RN: 87-61-6 **MP** (°C)**:** 51
MW: 181.45 **BP** (°C)**:** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-05	1.408E-02	20	K337	1 0 0 0 2	
6.607E-05	1.199E-02	22	K305	1 0 1 1 2	
8.983E-05	1.630E-02	23	C305	1 1 2 2 2	
9.920E-05	1.800E-02	25	B304	2 0 2 2 2	
1.170E-04	2.123E-02	25	B317	0 0 0 0 0	
9.920E-05	1.800E-02	25	C313	0 0 0 0 0	
6.760E-05	1.227E-02	25	M342	1 0 1 1 2	
9.149E-05	1.660E-02	ns	H123	0 0 0 0 0	
6.760E-05	1.227E-02	ns	M308	0 0 1 1 2	

583. $C_6H_3Cl_3$
1,3,5-Trichlorobenzene
Benzene, 1,3,5-trichloro-
RN: 108-70-3 **MP** (°C)**:** 64
MW: 181.45 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-05	4.353E-03	20	K337	1 0 0 0 2	
3.236E-05	5.872E-03	22	K305	1 0 1 1 2	
5.842E-05	1.060E-02	23	C305	1 1 2 2 2	
3.312E-05	6.010E-03	25	B304	2 0 2 2 2	
2.900E-05	5.262E-03	25	B317	0 0 0 0 0	
2.270E-05	4.119E-03	25	M342	1 0 1 1 2	
2.270E-05	4.119E-03	ns	M308	0 0 1 1 2	

584. $C_6H_3Cl_3$
1,2,4-Trichlorobenzene
Benzene, 1,2,4-trichloro-
RN: 120-82-1 **MP** (°C)**:** 17
MW: 181.45 **BP** (°C)**:** 213

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	3.000E-02	19	M172	1 0 0 0 0	
1.950E-04	3.538E-02	20	K337	1 0 0 0 2	
1.072E-04	1.944E-02	22	K305	1 0 1 1 2	
1.725E-04	3.130E-02	25	B304	2 0 2 2 2	
2.200E-04	3.992E-02	25	B317	0 0 0 0 0	
2.692E-04	4.884E-02	25	C113	1 0 2 2 2	
2.540E-04	4.609E-02	25	M342	1 0 1 1 2	
3.555E-04	6.451E-02	30	M300	1 1 2 2 2	
3.555E-04	6.450E-02	30	M311	1 1 2 2 2	
2.540E-04	4.609E-02	ns	M308	0 0 1 1 2	

585. $C_6H_3Cl_3N_2O_2$
Picloram
4-Amino-3,5,6-trichloropicolinic acid
RN: 1918-02-1 **MP** (°C)**:** 241
MW: 241.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.967E-03	4.750E-01	10	C031	2 0 2 2 2	pH 2.8
2.260E-03	5.457E-01	20	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	25	B185	0 0 0 0 0	
1.781E-03	4.300E-01	25	B200	1 0 0 0 1	
1.781E-03	4.300E-01	25	M161	1 0 0 0 2	
2.830E-03	6.833E-01	30	C031	2 0 2 2 2	pH 2.8
3.290E-03	7.944E-01	40	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	ns	K138	0 0 0 0 1	
1.780E-03	4.298E-01	ns	M061	0 0 0 0 1	
3.500E-04	8.451E-02	ns	O025	2 2 2 2 1	intrinsic

586. $C_6H_3Cl_3O$
2,3,4-Trichlorophenol
2,3,4-Trichlorphenol
RN: 15950-66-0 **MP** (°C)**:** 80
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-03	9.150E-01	25	M373	1 0 2 1 2	
2.138E-03	4.221E-01	ns	R424	0 0 0 0 0	

587. $C_6H_3Cl_3O$
2,3,5-Trichlorophenol
2,3,5-Trichlorphenol
RN: 933-78-8 **MP** (°C)**:** 62
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.905E-03	7.710E-01	25	M373	1 0 2 1 2	

588. $C_6H_3Cl_3O$
2,3,6-Trichlorophenol
2,3,6-Trichlorphenol
RN: 933-75-5 **MP** (°C)**:** 58
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.993E-03	5.910E-01	25	M373	1 0 2 1 2	

589. $C_6H_3Cl_3O$
2,4,6-Trichlorophenol
2,4,6-Trichlorphenol
Dowicide 25
RN: 88-06-2 **MP** (°C)**:** 69
MW: 197.45 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-03	5.000E-01	11.20	F300	1 0 0 0 0	
2.076E-03	4.100E-01	19.5	A400	2 1 2 2 2	
2.163E-03	4.270E-01	20.1	A400	2 1 2 2 2	
4.558E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.505E-03	6.920E-01	24.9	A400	2 1 2 2 2	
2.200E-03	4.344E-01	25	B316	0 0 0 0 0	
3.586E-03	7.080E-01	25	M373	1 0 2 1 2	
4.554E-03	8.992E-01	25	R041	0 0 0 0 0	
4.558E-03	9.000E-01	25.40	F300	1 0 0 0 0	

(*continued*)

589. $C_6H_3Cl_3O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.077E-02	6.075E+00	29.8	A400	2 1 2 2 2	
3.292E-02	6.501E+00	35.1	A400	2 1 2 2 2	
1.266E-02	2.500E+00	96	F300	1 0 0 0 1	
<5.06E-03	<9.99E-01	ns	N034	0 0 0 0 0	
3.981E-03	7.861E-01	ns	R427	0 0 0 0 0	

590. $C_6H_3Cl_3O$
2,4,5-Trichloro-phenol
Phenol, 2,4,5-trichloro-
Dowicide 2
Preventol I
2,4,5-Trichlorophenol
Collunosol
RN: 95-95-4 **MP** (°C)**:** 69
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-03	9.478E-01	25	B316	0 0 0 0 0	
3.287E-03	6.490E-01	25	M373	1 0 2 1 2	

591. $C_6H_3Cl_4N$
Nitrapyrin
2-Chloro-6-(trichloromethyl)pyridine
Donco-163
N-Serve(R)
RN: 1929-82-4 **MP** (°C)**:** 62.5
MW: 230.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.738E-04	4.013E-02	20	B179	0 0 0 0 0	
1.732E-04	4.000E-02	20	G079	1 1 0 0 2	
3.118E-04	7.200E-02	ns	V414	0 0 0 0 0	

592. $C_6H_3FN_2O_4$
1-Fluoro-2,4-dinitrobenzene
FDNB
RN: 70-34-8 **MP** (°C)**:** 26
MW: 186.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.149E-03	4.000E-01	ns	B160	0 0 0 0 2	

593. $C_6H_3F_3O$
Trifluorophenol
2,3,4-Trifluorophenol
RN: 2822-41-5 **MP** (°C)**:**
MW: 148.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	6.220E+01	25	P031	0 0 0 0 0	

594. $C_6H_3N_3O_6$
sym-Trinitrobenzene
1,3,5-Trinitro-benzol
1,3,5-Trinitrobenzene
RN: 99-35-4 **MP** (°C)**:** 122.5
MW: 213.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	2.780E-01	15	D066	1 2 0 0 2	
1.304E-03	2.779E-01	15	D070	1 2 0 0 2	
1.314E-03	2.800E-01	15	F300	1 0 0 0 1	
1.678E-03	3.577E-01	25	H434	0 0 0 0 0	
4.786E-03	1.020E+00	50	D066	1 2 0 0 2	
4.781E-03	1.019E+00	50	D070	1 2 0 0 2	
2.337E-02	4.980E+00	100	D066	1 2 0 0 2	
2.325E-02	4.955E+00	100	D070	1 2 0 0 2	
2.393E-02	5.100E+00	100	F300	1 0 0 0 1	
1.288E-03	2.745E-01	ns	R427	0 0 0 0 0	

595. $C_6H_3N_3O_7$
Picric acid
2,4,6-Trinitrophenol
Picronitric acid
Pikrinsaeure
RN: 88-89-1 **MP** (°C)**:** 122.5
MW: 229.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.948E-02	6.754E+00	0	D077	1 0 0 1 1	
4.322E-02	9.901E+00	0	M043	1 0 0 0 1	
4.364E-02	9.999E+00	7.10	E032	1 2 1 2 2	
4.232E-02	9.695E+00	9	D080	1 2 0 0 2	unit assumed
3.507E-02	8.035E+00	10	D077	1 0 0 1 1	
4.749E-02	1.088E+01	10	M043	1 0 0 0 1	
4.407E-02	1.010E+01	18.90	E032	1 2 1 2 2	
4.792E-02	1.098E+01	20	D077	1 0 0 1 2	
5.151E-02	1.180E+01	20	H048	1 0 0 0 2	unit assumed
4.300E-02	9.852E+00	20	K310	1 0 0 1 1	

(*continued*)

595. $C_6H_3N_3O_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-02	1.186E+01	20	M043	1 0 0 0 1	
4.932E-02	1.130E+01	23.50	F300	0 0 0 0 2	
5.327E-02	1.220E+01	25	D058	1 0 1 1 2	
5.520E-02	1.265E+01	25	F030	1 0 2 1 2	
5.684E-02	1.302E+01	25	H048	1 0 0 0 2	unit assumed
5.780E-02	1.324E+01	25	K040	1 0 2 1 2	
5.474E-02	1.254E+01	25	M094	1 0 0 1 2	
6.026E-02	1.381E+01	30	D077	1 0 0 1 2	
6.450E-02	1.478E+01	30	M043	1 0 0 0 1	
7.465E-02	1.710E+01	33.30	E032	1 2 1 2 2	
7.633E-02	1.749E+01	40	D077	1 0 0 1 2	
8.138E-02	1.865E+01	40	M043	1 0 0 0 1	
9.396E-02	2.153E+01	44.30	E032	1 2 1 2 2	
9.354E-02	2.143E+01	50	D077	1 0 0 1 2	
9.930E-02	2.275E+01	50	D080	1 2 0 0 2	unit assumed
1.193E-01	2.733E+01	60	D077	1 0 0 1 2	
1.312E-01	3.007E+01	60	M043	1 0 0 0 1	
1.398E-01	3.204E+01	62.90	E032	1 2 1 2 2	
1.464E-01	3.354E+01	70	D077	1 0 0 1 2	
1.703E-01	3.902E+01	72.60	E032	1 2 1 2 2	
1.844E-01	4.224E+01	80	D077	1 0 0 1 2	
1.920E-01	4.398E+01	80	M043	1 0 0 0 1	
1.956E-01	4.481E+01	82	D080	1 2 0 0 2	unit assumed
2.007E-01	4.598E+01	83.90	E032	1 2 1 2 2	
2.362E-01	5.411E+01	90	D077	1 0 0 1 2	
2.160E-01	4.949E+01	90	K310	1 0 0 1 2	
2.244E-01	5.141E+01	90.10	E032	1 2 1 2 2	
2.326E-01	5.330E+01	92.40	E032	1 2 1 2 2	
2.517E-01	5.767E+01	94.80	E032	1 2 1 2 2	
2.947E-01	6.751E+01	100	D077	1 0 0 1 2	
3.083E-01	7.063E+01	100	D080	1 2 0 0 2	unit assumed
3.055E-01	7.000E+01	100	F300	1 0 0 0 1	
2.932E-01	6.716E+01	100	M043	1 0 0 0 1	

596. $C_6H_3N_3O_8$

Styphnic acid
Styphninsaeure

RN: 82-71-3 **MP** (°C)**:** 176
MW: 245.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-02	5.865E+00	6.10	E032	1 2 1 2 2	
2.167E-02	5.312E+00	16.60	E032	1 2 1 2 2	
2.203E-02	5.400E+00	25	F300	1 0 0 0 1	
2.179E-02	5.341E+00	25	K040	1 0 2 1 2	
2.997E-02	7.346E+00	35.70	E032	1 2 1 2 2	
3.471E-02	8.507E+00	47.10	E032	1 2 1 2 2	

(*continued*)

596. $C_6H_3N_3O_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.119E-02	1.010E+01	56.90	E032	1 2 1 2 2	
4.692E-02	1.150E+01	62	F300	1 0 0 0 2	
4.758E-02	1.166E+01	63.00	E032	1 2 1 2 2	
6.109E-02	1.497E+01	71.20	E032	1 2 1 2 2	
7.135E-02	1.749E+01	76.20	E032	1 2 1 2 2	
8.000E-02	1.961E+01	80.30	E032	1 2 1 2 2	
9.562E-02	2.344E+01	85.00	E032	1 2 1 2 2	
1.096E-01	2.686E+01	89.80	E032	1 2 1 2 2	
1.357E-01	3.326E+01	95.90	E032	1 2 1 2 2	

597. C_6H_4BrF

1-Bromo-2-fluorobenzene
2-Bromofluorobenzene

RN: 1072-85-1 **MP** (°C)**:**
MW: 175.01 **BP** (°C)**:** 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.018E-03	3.532E-01	25	B349	2 0 2 0 2	

598. C_6H_4BrF

1-Bromo-3-fluorobenzene
3-Bromofluorobenzene

RN: 1073-06-9 **MP** (°C)**:**
MW: 175.01 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.162E-03	3.784E-01	25	B349	2 0 2 0 2	

599. $C_6H_4BrNO_3$

2-Bromo-4-nitrophenol
2-Brom-4-nitro-phenol

RN: 5847-59-6 **MP** (°C)**:** 114
MW: 218.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	2.200E+01	100	F300	1 0 0 0 1	

600. $C_6H_4Br_2$
m-Dibromobenzene
1,3-Dibromobenzene
RN: 108-36-1 **MP** (°C)**:** –7
MW: 235.92 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-04	6.747E-02	35	H077	2 2 2 2 2	

601. $C_6H_4Br_2$
p-Dibromobenzene
1,4-Dibromobenzene
RN : 106-37-6 **MP** (°C)**:** 87.3
MW: 235.92 **BP** (°C)**:** 220.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-05	9.910E-03	10	K440	0 0 0 0 0	
8.478E-05	2.000E-02	25	A003	1 0 1 2 1	
5.900E-03	1.392E+00	25	C316	0 0 0 0 0	0.1M NaCl
7.206E-05	1.700E-02	25	K440	0 0 0 0 0	
1.120E-04	2.642E-02	35	H077	2 2 2 2 2	
1.043E-04	2.460E-02	35	K440	0 0 0 0 0	

602. C_6H_4ClF
1-Chloro-2-fluorobenzene
2-Chlorofluorobenzene
RN: 348-51-6 **MP** (°C)**:** –43
MW: 130.55 **BP** (°C)**:** 137.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-03	5.019E-01	25	B349	2 0 2 0 2	

603. C_6H_4ClF
1-Chloro-3-fluorobenzene
3-Chlorofluorobenzene
RN: 625-98-9 **MP** (°C)**:**
MW: 130.55 **BP** (°C)**:** 127.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.517E-03	5.897E-01	25	B349	2 0 2 0 2	

604. $C_6H_4ClIO_2S$

Pipsyl chloride
p-Iodobenzenesulfonyl chloride
RN: 98-61-3 **MP** (°C)**:** 81
MW: 302.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.388E-05	1.630E-02	25	B048	1 0 2 2 2	
8.793E-05	2.660E-02	35	B048	1 0 2 2 2	
1.646E-04	4.980E-02	50	B048	1 0 2 2 2	

605. $C_6H_4ClNO_2$

6-Chloropicolinic acid
Pyridinecarboxylic acid, 6-chloro-
RN: 4684-94-0 **MP** (°C)**:**
MW: 157.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.158E-02	3.400E+00	ns	K138	0 0 0 0 1	
2.138E-02	3.369E+00	ns	R427	0 0 0 0 0	

606. $C_6H_4ClNO_2$

p-Chloronitrobenzene
4-Nitrochlorobenzene
4-CNB
4-Chloronitrobenzene
RN: 100-00-5 **MP** (°C)**:** 82
MW: 157.56 **BP** (°C)**:** 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.711E-04	1.530E-01	9.99	B403	1 2 2 2 2	
1.777E-04	2.800E-02	17	D071	1 2 0 0 1	
1.777E-04	2.800E-02	17	F300	1 0 0 0 1	
1.327E-03	2.090E-01	19.99	B403	1 2 2 2 2	
2.877E-03	4.533E-01	20	E308	1 2 2 1 2	
1.429E-03	2.251E-01	20	H118	1 1 1 1 2	
1.429E-03	2.251E-01	20	H301	0 0 0 0 0	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.600E-03	2.521E-01	25	G090	2 2 1 1 1	
1.739E-03	2.740E-01	29.99	B403	1 2 2 2 2	
2.348E-03	3.700E-01	39.99	B403	1 2 2 2 2	
7.933E-04	1.250E-01	50	D071	1 2 0 0 2	
9.709E-04	1.530E-01	100	D071	1 2 0 0 2	
1.016E-03	1.600E-01	100	F300	1 0 0 0 2	

607. $C_6H_4ClNO_2$

m-Chloronitrobenzene
1-Chloro-3-nitrobenzene
3-Chloronitrobenzene
m-Nitrochlorobenzene

RN: 121-73-3 **MP** (°C)**:** 46.0
MW: 157.56 **BP** (°C)**:** 236.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.732E-03	2.729E-01	20	E308	1 2 2 1 2	

608. $C_6H_4ClNO_2$

o-Chloronitrobenzene
2-Nitrochlorobenzene
2-CNB
1-Chloro-2-nitrobenzene

RN: 88-73-3 **MP** (°C)**:** 32
MW: 157.56 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-03	2.280E-01	9.99	B403	1 2 2 2 2	
2.133E-03	3.360E-01	19.99	B403	1 2 2 2 2	
2.800E-03	4.412E-01	20	E308	1 2 2 1 2	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
3.470E-03	5.467E-01	25	G090	2 2 1 1 1	
3.199E-03	5.040E-01	29.99	B403	1 2 2 2 2	
4.271E-03	6.730E-01	39.99	B403	1 2 2 2 2	

609. $C_6H_4Cl_2$

1,2-Dichlorobenzene
o-Dichlorobenzene

RN: 95-50-1 **MP** (°C)**:** –17
MW: 147.00 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.047E-04	1.330E-01	3.5	C094	1 0 0 0 2	
1.007E-03	1.480E-01	20	C094	1 0 0 0 2	
9.114E-04	1.340E-01	20	K056	1 0 2 2 2	
9.550E-04	1.404E-01	20	K337	1 0 0 0 2	
6.607E-04	9.713E-02	22	K305	1 0 1 1 2	
<1.36E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.060E-03	1.558E-01	25	B173	2 0 2 2 2	
9.864E-04	1.450E-01	25	B185	0 0 0 0 0	
9.319E-04	1.370E-01	25	B304	2 0 2 2 2	
8.000E-04	1.176E-01	25	B317	0 0 0 0 0	
1.047E-03	1.539E-01	25	C113	1 0 2 2 2	
9.864E-04	1.450E-01	25	K056	1 0 2 2 2	
1.156E-03	1.700E-01	25	L319	1 0 2 1 1	
6.280E-04	9.232E-02	25	M342	1 0 1 1 2	
1.163E-03	1.710E-01	30	K056	1 0 2 2 2	

(*continued*)

609. $C_6H_4Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.016E-03	1.494E-01	30	M300	1 1 2 2 2	
9.680E-04	1.423E-01	30	M311	1 1 2 2 2	
1.245E-03	1.830E-01	35	K056	1 0 2 2 2	
1.320E-03	1.940E-01	40	K056	1 0 2 2 2	
1.381E-03	2.030E-01	45	K056	1 0 2 2 2	
1.517E-03	2.230E-01	55	K056	1 0 2 2 2	
1.578E-03	2.320E-01	60	K056	1 0 2 2 2	
1.060E+03	1.558E+05	ns	A096	0 0 0 0 2	*sic*
6.280E-04	9.232E-02	ns	M308	0 0 1 1 2	

610. $C_6H_4Cl_2$

1,3-Dichlorobenzene
m-Dichlorobenzene

RN: 541-73-1 **MP** (°C)**:** –24
MW: 147.00 **BP** (°C)**:** 172–173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-04	1.110E-01	20	K056	1 0 2 2 2	
7.943E-04	1.168E-01	20	K337	1 0 0 0 2	
4.677E-04	6.876E-02	22	K305	1 0 1 1 2	
9.080E-04	1.335E-01	25	B173	2 0 2 2 2	
9.728E-04	1.430E-01	25	B304	2 1 2 1 2	
8.300E-04	1.220E-01	25	B317	0 0 0 0 0	
9.120E-04	1.341E-01	25	C113	1 0 2 2 2	
8.367E-04	1.230E-01	25	K056	1 0 2 2 2	
8.470E-04	1.245E-01	25	M342	1 0 1 1 2	
9.523E-04	1.400E-01	30	K056	1 0 2 2 2	
8.537E-04	1.255E-01	30	M300	1 1 2 2 2	
8.537E-04	1.255E-01	30	M311	1 1 2 2 2	
1.020E-03	1.500E-01	35	K056	1 0 2 2 2	
1.136E-03	1.670E-01	40	K056	1 0 2 2 2	
1.204E-03	1.770E-01	45	K056	1 0 2 2 2	
1.333E-03	1.960E-01	55	K056	1 0 2 2 2	
1.367E-03	2.010E-01	60	K056	1 0 2 2 2	
9.080E+02	1.335E+05	ns	A096	0 0 0 0 2	*sic*
8.470E-04	1.245E-01	ns	M308	0 0 1 1 2	

611. $C_6H_4Cl_2$

1,4-Dichlorobenzene
p-Dichlorobenzene

RN: 106-46-7 **MP** (°C)**:** 53.1
MW: 147.00 **BP** (°C)**:** 173.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-04	6.880E-02	20	K056	1 2 2 1 2	average of 4
3.020E-04	4.439E-02	20	K337	1 0 0 0 2	
2.252E-04	3.310E-02	20	T301	1 2 2 2 2	

(*continued*)

611. $C_6H_4Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	4.868E-02	22	K305	1 0 1 1 2	
5.292E-04	7.780E-02	22.20	W003	2 2 2 2 2	average of 2
5.673E-04	8.340E-02	24.60	W003	2 2 2 2 2	average of 3
5.170E-04	7.600E-02	25	A003	1 0 1 2 1	
5.928E-04	8.715E-02	25	A058	1 1 1 1 2	
<3.40E-03	<5.00E-01	25	B019	1 0 1 2 0	
5.020E-04	7.380E-02	25	B173	2 0 2 2 2	
4.442E-04	6.530E-02	25	B304	2 0 2 2 2	
5.270E-04	7.747E-02	25	B317	0 0 0 0 0	
3.990E-04	5.865E-02	25	C316	0 0 0 0 0	0.1M NaCl
5.374E-04	7.900E-02	25	F071	1 1 2 1 1	
5.374E-04	7.900E-02	25	H080	1 0 0 0 1	
5.381E-04	7.910E-02	25	K056	1 2 2 2 2	average of 2
5.646E-04	8.300E-02	25	M040	1 0 0 1 1	
5.442E-04	8.000E-02	25	M161	1 0 0 0 1	
2.100E-04	3.087E-02	25	M342	1 0 1 1 2	
6.932E-05	1.019E-02	25	N311	1 0 1 1 2	
4.100E-04	6.027E-02	25.2	T428	0 0 0 0 0	
5.898E-04	8.670E-02	25.50	W003	2 2 2 2 2	average of 2
5.238E-04	7.699E-02	30	G029	1 0 2 2 1	
6.347E-04	9.330E-02	30	K056	1 2 2 2 2	
6.267E-04	9.213E-02	30	M300	1 1 2 2 2	
6.422E-04	9.440E-02	30	M311	1 1 2 2 2	
6.299E-04	9.260E-02	30.00	W003	2 2 2 2 2	average of 2
6.939E-04	1.020E-01	34.50	W003	2 2 2 2 2	average of 3
5.646E-04	8.300E-02	35	K056	1 2 2 2 2	
8.231E-04	1.210E-01	38.40	W003	2 2 2 2 2	
6.857E-04	1.008E-01	40	K056	1 2 2 2 2	average of 2
8.292E-04	1.219E-01	45	K056	1 2 2 2 2	average of 2
1.082E-03	1.590E-01	47.50	W003	2 2 2 2 2	
1.184E-03	1.740E-01	50.10	W003	2 2 2 2 2	average of 2
1.061E-03	1.560E-01	55	K056	1 2 2 2 2	
1.429E-03	2.100E-01	59.20	W003	2 2 2 2 2	
1.109E-03	1.630E-01	60	K056	1 2 2 2 2	
1.483E-03	2.180E-01	60.70	W003	2 2 2 2 2	average of 2
1.565E-03	2.300E-01	65.10	W003	2 2 2 2 2	average of 3
1.612E-03	2.370E-01	65.20	W003	2 2 2 2 2	average of 3
1.912E-03	2.810E-01	73.40	W003	2 2 2 2 2	
2.100E-04	3.087E-02	ns	M308	0 0 1 1 2	
5.374E-04	7.900E-02	ns	M344	0 0 0 0 1	
5.034E-04	7.400E-02	rt	S314	0 0 2 1 1	

612. $C_6H_4Cl_2N_2O_2$

Dicloran

RN: 99-30-9 **MP** (°C)**:** 195
MW: 207.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-05	6.252E-03	ns	R424	0 0 0 0 0	
3.020E-05	6.252E-03	ns	R427	0 0 0 0 0	

613. $C_6H_4Cl_2O$
2,4-Dichlorophenol
2,4-Dichlor-phenol
RN: 120-83-2 **MP** (°C)**:** 45
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.390E-02	3.896E+00	15.3	A400	2 1 2 2 2	
2.748E-02	4.480E+00	19	D041	1 0 0 0 1	
~2.76E-02	~4.50E+00	20	F300	1 0 0 0 0	
2.748E-02	4.480E+00	20	N034	1 0 0 0 1	
3.403E-02	5.547E+00	25	M373	1 0 2 1 2	
3.052E-02	4.975E+00	25	R041	0 0 0 0 0	
3.385E-02	5.517E+00	25.2	A400	2 1 2 2 2	
1.748E-01	2.850E+01	34.6	A400	2 1 2 2 2	
2.754E-02	4.490E+00	ns	R427	0 0 0 0 0	

614. $C_6H_4Cl_2O$
3,5-Dichlorophenol
3,5-DCP
RN: 591-35-5 **MP** (°C)**:** 68
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-02	7.394E+00	25	M373	1 0 2 1 2	

615. $C_6H_4Cl_2O$
3,4-Dichlorophenol
4,5-Dichlorophenol
3,4-DCP
RN: 95-77-2 **MP** (°C)**:** 67
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-02	9.256E+00	25	M373	1 0 2 1 2	

616. $C_6H_4Cl_2O$
2,6-Dichlorophenol
2,6-DCP
RN: 87-65-0 **MP** (°C)**:** 66.5
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-02	2.625E+00	25	M373	1 0 2 1 2	

617. $C_6H_4Cl_2O$
2,3-Dichlorophenol
Phenol, 2,3-dichloro-
RN: 576-24-9 **MP** (°C)**:** 59
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.040E-02	8.215E+00	25	M373	1 0 2 1 2	

618. $C_6H_4Cl_2O$
2,5-Dichlorophenol
2,5-Dichlor-phenol
RN: 583-78-8 **MP** (°C)**:**
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-02	6.194E+00	25	B316	0 0 0 0 0	

619. C_6H_4FI
1-Fluoro-4-iodobenzene
4-Fluoro-1-iodobenzene
p-Iodofluorobenzene
p-Fluoroiodobenzene
p-Fluorophenyl iodide
RN: 352-34-1 **MP** (°C)**:** –27
MW: 222.00 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-04	1.665E-01	25	B349	2 0 2 0 2	

620. $C_6H_4I_2$
1,4-Diiodobenzene
p-Diiodobenzene
4-Iodophenyl iodide
RN: 624-38-4 **MP** (°C)**:** 131
MW: 329.91 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.244E-06	1.400E-03	25	A003	1 2 1 2 1	*sic*
3.100E-02	1.023E+01	25	C316	0 0 0 0 0	0.1M NaCl

621. $C_6H_4N_2O_4$
p-Dinitrobenzene
1,4-Dinitrobenzene
RN: 100-25-4 **MP** (°C)**:** 173
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.759E-04	8.000E-02	20	F300	1 0 0 0 0	
2.350E-04	3.951E-02	25	C316	0 0 0 0 0	0.1M NaCl
4.090E-04	6.876E-02	25	I334	2 2 2 1 2	
3.676E-04	6.180E-02	25	L008	2 2 2 1 2	average of 2
6.170E-04	1.037E-01	35	H077	2 2 2 2 2	
1.130E-02	1.900E+00	100	F300	1 0 0 0 1	

622. $C_6H_4N_2O_4$
m-Dinitrobenzene
1,3-Dinitrobenzene
RN: 99-65-0 **MP** (°C)**:** 89.5
MW: 168.11 **BP** (°C)**:** 301.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.045E-04	6.800E-02	13	D070	1 2 0 0 1	
4.164E-04	7.000E-02	13	F300	1 0 0 0 0	
3.420E-03	5.749E-01	25	I334	2 2 2 1 2	
3.169E-03	5.328E-01	25	L008	2 2 2 1 2	average of 2
5.116E-03	8.600E-01	25.04	V013	2 2 2 2 2	
3.867E-03	6.500E-01	30	F300	1 0 0 0 1	
3.888E-03	6.536E-01	30	G029	1 0 2 2 2	
4.670E-03	7.851E-01	35	H077	2 2 2 2 2	
2.789E-03	4.688E-01	50	D070	1 2 0 0 2	
1.134E-02	1.906E+00	100	D070	1 2 0 0 2	
1.547E-02	2.600E+00	100	F300	1 0 0 0 1	
2.973E-03	4.998E-01	rt	D021	0 0 1 1 0	

623. $C_6H_4N_2O_4$
o-Dinitrobenzene
1,2-Dinitrobenzene
RN: 528-29-0 **MP** (°C)**:** 118
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.328E-04	1.400E-01	20	F300	1 0 0 0 1	
7.910E-04	1.330E-01	25	I334	2 2 2 1 2	
7.418E-04	1.247E-01	25	L008	2 2 2 1 2	average of 3

624. $C_6H_4N_2O_5$
3,5-Dinitrophenol
Phenol, θ-dinitro-
RN: 586-11-8 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.288E-02	1.342E+01	51.6	S117	1 2 1 1 2	solid hydrate
2.373E+00	4.370E+02	54.1	S117	1 2 1 1 2	anhydrate
2.407E+00	4.431E+02	54.5	S117	1 2 1 1 2	anhydrate
2.442E+00	4.496E+02	55.5	S117	1 2 1 1 2	anhydrate
2.474E+00	4.555E+02	57.9	S117	1 2 1 1 2	anhydrate
2.516E+00	4.633E+02	61.9	S117	1 2 1 1 2	anhydrate
2.583E+00	4.756E+02	69.9	S117	1 2 1 1 2	anhydrate
2.617E+00	4.819E+02	81.3	S117	1 2 1 1 2	anhydrate
5.308E-01	9.772E+01	109.3	S117	1 0 1 1 2	
1.253E+00	2.307E+02	124.6	S117	1 0 1 1 2	

625. $C_6H_4N_2O_5$
2,6-Dinitrophenol
β-Dinitrophenol
RN: 573-56-8 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-03	3.149E-01	15	D080	1 2 0 0 2	unit assumed
1.629E-03	3.000E-01	15	F300	1 0 0 0 0	
2.805E-02	5.164E+00	50	D080	1 2 0 0 2	unit assumed
6.547E-02	1.205E+01	100	D080	1 2 0 0 2	unit assumed
6.518E-02	1.200E+01	100	F300	1 0 0 0 1	

626. $C_6H_4N_2O_5$
2,4-Dinitrophenol
α-Dinitrophenol
Aldifen
Fenoxyl carbon N
RN: 51-28-5 **MP** (°C)**:** 107.5
MW: 184.11 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.097E-03	2.020E-01	12.5	D069	1 2 0 0 2	
1.086E-03	2.000E-01	12.50	F300	1 0 0 0 0	
1.629E-03	2.999E-01	15	D079	1 2 0 0 1	
2.254E-03	4.150E-01	15.1	A400	2 1 2 2 2	
3.025E-02	5.569E+00	18	D041	1 0 0 0 1	
2.800E-02	5.155E+00	20	K301	2 2 1 1 1	
2.524E-03	4.647E-01	25	H085	2 0 2 1 2	

(*continued*)

626. $C_6H_4N_2O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.467E-03	2.700E-01	25	P037	2 0 1 1 2	
3.753E-03	6.910E-01	25.0	A400	2 1 2 2 2	
1.901E-01	3.500E+01	35.0	A400	2 1 2 2 2	
4.356E-03	8.020E-01	50	D069	1 2 0 0 2	
9.504E-04	1.750E-01	50	D079	1 2 0 0 2	
7.431E-03	1.368E+00	54.50	E032	1 2 1 2 2	
1.192E-02	2.195E+00	67.60	E032	1 2 1 2 2	
1.630E-02	3.001E+00	75.80	E032	1 2 1 2 2	
3.414E-02	6.286E+00	85	D069	1 2 0 0 2	
3.170E-02	5.836E+00	87.40	E032	1 2 1 2 2	
4.845E-02	8.920E+00	92.40	E032	1 2 1 2 2	
6.547E-02	1.205E+01	96.20	E032	1 2 1 2 2	
7.163E-02	1.319E+01	100	D069	1 2 0 0 2	
8.964E-02	1.650E+01	100	D079	1 2 0 0 2	
7.061E-02	1.300E+01	100	F300	1 0 0 0 1	
2.444E-01	4.500E+01	h	F300	0 0 0 0 1	
2.702E-02	4.975E+00	ns	M061	0 0 0 0 0	

627. $C_6H_4N_2O_6$

2,4-Dinitroresorcinol
2,4-Dinitro-1,3-benzenediol

RN: 519-44-8 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-02	6.261E+00	57.70	E032	1 2 1 2 2	
4.801E-02	9.607E+00	66.60	E032	1 2 1 2 2	
7.434E-02	1.488E+01	69.50	E032	1 2 1 2 2	
9.895E-02	1.980E+01	76.50	E032	1 2 1 2 2	
1.690E-01	3.382E+01	84.70	E032	1 2 1 2 2	
2.380E-01	4.762E+01	90.00	E032	1 2 1 2 2	
3.495E-01	6.994E+01	93.00	E032	1 2 1 2 2	

628. $C_6H_4N_2O_6$

4,6-Dinitroresorcinol
4,6-Dinitro-1,3-benzenediol

RN: 616-74-0 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	3.998E-01	77.00	E032	1 2 1 2 2	
3.995E-03	7.994E-01	90.50	E032	1 2 1 2 2	
4.992E-03	9.990E-01	96.30	E032	1 2 1 2 2	

629. $C_6H_4N_4$
Pteridine
1,3,5,8-Tetraazanaphthalene
Azinepurine
Pyrimido[4,5-b]pyrazine
Pyrazino[2,3-d]pyrimidine
RN: 91-18-9 **MP** (°C)**:** 138
MW: 132.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.461E-01	1.250E+02	20	A020	1 2 0 0 1	
9.461E-01	1.250E+02	20	B050	1 0 0 0 0	
9.230E-01	1.220E+02	22.5	A085	1 2 0 0 0	
3.784E+00	5.000E+02	100	B050	1 0 0 0 0	

630. $C_6H_4N_4O$
4-Hydroxypteridine
4-Pteridinol
RN: 700-47-0 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-02	4.975E+00	20	A020	1 2 0 0 1	
3.359E-02	4.975E+00	20	B050	1 0 0 0 0	
3.359E-02	4.975E+00	22.5	A085	1 2 0 0 0	
2.250E-01	3.333E+01	100	B050	1 0 0 0 0	

631. $C_6H_4N_4O$
6-Hydroxypteridine
6-Pteridinol
RN: 2432-26-0 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-03	2.856E-01	20	A020	1 2 0 0 1	
1.928E-03	2.856E-01	20	B050	1 0 0 0 0	
2.923E-02	4.329E+00	100	B050	1 0 0 0 0	

632. $C_6H_4N_4O$
7-Hydroxypteridine
7-Pteridinol
RN: 2432-27-1 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.493E-03	1.110E+00	20	B050	1 0 0 0 0	
8.768E-02	1.299E+01	100	B050	1 0 0 0 0	

633. $C_6H_4N_4O$
2-Hydroxypteridine
2-Pteridinol
RN: 25911-76-6 **MP** (°C)**:** 240
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.664E+00	20	A020	1 2 0 0 1	
1.123E-02	1.664E+00	20	B050	1 0 0 0 0	
1.123E-02	1.664E+00	22.5	A085	1 2 0 0 0	
1.324E-01	1.961E+01	100	B050	1 0 0 0 0	

634. $C_6H_4N_4O_2$
2,4-Dihydroxypteridine
2:4-Dihydroxypteridine
Lumazine
RN: 487-21-8 **MP** (°C)**:** 348.5
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.607E-03	1.248E+00	20	B050	1 0 0 0 0	
7.607E-03	1.248E+00	22.5	A085	1 2 0 0 0	
5.035E-02	8.264E+00	100	B050	1 0 0 0 0	

635. $C_6H_4N_4O_2$
2,7-Dihydroxypteridine
2:7-Dihydroxypteridine
RN: 65882-62-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.033E-02	9.901E+00	100	A020	1 2 0 0 0	

636. $C_6H_4N_4O_2$
4,6-Dihydroxypteridine
4:6-Dihydroxypteridine
RN: 16310-36-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.108E-03	1.818E-01	20	A020	1 2 0 0 1	
1.218E-03	2.000E-01	20	B050	1 0 0 0 0	
2.024E-02	3.322E+00	100	B050	1 0 0 0 0	

637. $C_6H_4N_4O_2$
4,7-Dihydroxypteridine
4:7-Dihydroxypteridine
6,7-Dihydroxypteridine
6:7-Dihydroxypteridine
RN: 33669-70-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	3.332E-01	20	A020	1 2 0 0 1	
1.523E-03	2.499E-01	20	A020	1 2 0 0 1	
2.030E-03	3.332E-01	20	B050	1 0 0 0 0	
1.523E-03	2.499E-01	20	B050	1 0 0 0 0	
2.094E-02	3.436E+00	100	B050	1 0 0 0 0	
1.014E-02	1.664E+00	100	B050	1 0 0 0 0	

638. $C_6H_4N_4O_2$
2,6-Dihydroxypteridine
2:6-Dihydroxypteridine
RN: 89324-38-9 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.222E-01	100	A020	1 2 0 0 1	

639. $C_6H_4N_4O_3$
2,4,7-Trihydroxypteridine
2:4:7-Trihydroxypteridine
RN: 2577-38-0 **MP** (°C)**:**
MW: 180.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.626E-04	8.333E-02	20	A020	1 2 0 1 1	
4.626E-04	8.333E-02	20	B050	1 0 0 0 0	
3.963E-03	7.138E-01	100	A020	1 2 0 0 1	
3.963E-03	7.138E-01	100	B050	1 0 0 0 0	

640. $C_6H_4N_4O_3$
4,6,7-Trihydroxypteridine
4:6:7-Trihydroxypteridine
RN: 58947-88-9 **MP** (°C)**:**
MW: 180.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-04	3.704E-02	20	A020	1 2 0 0 1	
2.056E-04	3.704E-02	20	B050	1 0 0 0 0	
7.930E-04	1.428E-01	100	B050	1 0 0 0 0	

641. $C_6H_4N_4O_4$
2,4,6,7-Tetrahydroxypteridine
2,4,6-Trihydroxypteridine
2:4:6-Trihydroxypteridine
RN: 2817-14-3 **MP** (°C)**:**
MW: 196.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.791E-05	1.724E-02	20	A020	1 2 0 1 1	
6.889E-04	1.351E-01	20	B050	1 0 0 0 0	
8.791E-05	1.724E-02	20	B050	1 0 0 0 0	
1.272E-02	2.494E+00	100	A020	1 2 0 0 0	
7.283E-04	1.428E-01	100	A020	1 2 0 0 0	
1.272E-02	2.494E+00	100	B050	1 0 0 0 0	

642. $C_6H_4N_4O_6$
Picramine
2,4,6-Trinitroaniline
1-Amino-2,4,6-trinitrobenzene
MATB
RN: 489-98-5 **MP** (°C)**:** 192
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-05	1.987E-02	25	B335	1 2 0 0 1	

643. $C_6H_4N_4S$
4-Mercaptopteridine
4-Pteridinethiol
4(1H)-Pteridinethione
Pteridine-4-thiol
RN: 65882-61-3 **MP** (°C)**:** 176dec
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.691E-03	2.777E-01	22.5	A085	1 2 0 0 0	

644. $C_6H_4N_4S$
2-Mercaptopteridine
2-Pteridinethiol
2(1H)-Pteridinethione
RN: 16878-76-5 **MP** (°C)**:** 205
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.347E-03	7.138E-01	22.5	A085	1 2 0 0 0	

645. $C_6H_4N_4S$
7-Mercaptopteridine
7-Pteridinethiol
7(1H)-Pteridinethione
RN: 36653-71-1 **MP** (°C)**:**
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-03	3.225E-01	20	A083	1 2 0 0 0	
6.760E-03	1.110E+00	100	A083	1 2 0 0 0	

646. $C_6H_4O_2$
Quinone
1,4-Benzoquinone
Benzochinhydrone
p-Quinone
RN: 106-51-4 **MP** (°C)**:** 115.7
MW: 108.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-02	9.329E+00	11.85	L064	2 2 2 1 2	0.01N HCl
1.013E-01	1.095E+01	17.70	L065	1 0 0 0 2	0.01N HCl
1.021E-01	1.104E+01	17.90	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	17.95	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	18	L064	2 2 2 1 2	0.01N HCl
1.580E-02	1.708E+00	20	B113	1 2 2 1 2	
1.233E-01	1.333E+01	23.85	L064	2 2 2 1 2	0.01N HCl
1.295E-01	1.400E+01	24	F300	1 0 0 0 1	
1.266E-01	1.369E+01	25	G033	1 0 1 1 2	
1.397E-01	1.510E+01	25	K033	1 0 0 1 2	

647. $C_6H_4O_5$
2,5-Dicarboxyfuran
Furan-dicarbon-saeure-(2,5)
RN: 3238-40-2 **MP** (°C)**:**
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.406E-03	1.000E+00	18	F300	1 0 0 0 0	

648. $C_6H_4O_5$
2-Carboxy-5-hydroxy-4-pyrone
Komensaeure
Komenic acid
RN: 499-78-5 **MP** (°C)**:**
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.267E-02	5.100E+00	25	F300	1 0 0 0 1	
3.921E-01	6.120E+01	100	F300	1 0 0 0 2	

649. C_6H_5Br
Bromobenzene
Phenyl bromide
Monobromobenzene
RN: 108-86-1 **MP** (°C)**:** –30
MW: 157.02 **BP** (°C)**:** 156.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.611E-03	4.100E-01	25	A003	1 2 1 2 1	
2.620E-03	4.114E-01	25	W300	2 2 2 2 2	
2.840E-03	4.460E-01	30	F071	1 1 2 1 2	
2.966E-03	4.658E-01	30	G029	1 0 2 2 2	
2.840E-03	4.460E-01	30	H080	1 0 0 0 2	
2.102E-03	3.300E-01	30	M311	1 1 2 2 2	
2.799E-03	4.395E-01	30	V009	1 0 0 0 1	
2.920E-03	4.585E-01	35	H077	2 2 2 2 2	
5.110E-04	8.024E-02	ns	D348	0 0 0 0 0	
2.615E-03	4.106E-01	ns	M344	0 0 0 0 2	

650. C_6H_5BrO
p-Bromophenol
4-Bromophenol
RN: 106-41-2 **MP** (°C)**:** 66
MW: 173.02 **BP** (°C)**:** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.053E-02	1.393E+01	20	R087	0 0 0 0 0	0.15M NaCl
8.542E-02	1.478E+01	25	R041	0 0 0 0 0	
8.128E-02	1.406E+01	ns	R424	0 0 0 0 0	

651. $C_6H_5BrO_3S$

p-Bromobenzenesulfonic acid
4-Bromobenzenesulfonic acid
RN: 138-36-3 **MP** (°C)**:**
MW: 237.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E+00	4.929E+02	82.3	T023	1 2 2 1 2	
2.088E+00	4.949E+02	89.6	T023	1 2 2 1 2	
2.093E+00	4.961E+02	93.1	T023	1 2 2 1 2	
2.097E+00	4.972E+02	97.6	T023	1 2 2 1 2	

652. $C_6H_5BrO_3S.H_2O$

p-Bromobenzenesulfonic acid (monohydrate)
RN: 138-36-3 **MP** (°C)**:**
MW: 255.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E+00	4.588E+02	43.8	T023	1 2 2 1 2	
1.821E+00	4.644E+02	60.2	T023	1 2 2 1 2	
1.586E+00	4.045E+02	71.2	T023	1 2 2 1 2	
1.924E+00	4.909E+02	76.6	T023	1 2 2 1 2	
1.922E+00	4.903E+02	78.5	T023	1 2 2 1 2	
1.855E+00	4.731E+02	80.3	T023	1 2 2 1 2	
1.868E+00	4.766E+02	86.2	T023	1 2 2 1 2	
1.907E+00	4.865E+02	87.2	T023	1 2 2 1 2	
1.889E+00	4.818E+02	90.2	T023	1 2 2 1 2	

653. $C_6H_5BrO_3S.2.5H_2O$

p-Bromobenzenesulfonic acid (2.5 hydrate)
RN: 138-36-3 **MP** (°C)**:**
MW: 282.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.375E+00	3.880E+02	–21.0	T023	1 2 2 1 2	
1.409E+00	3.975E+02	–10.5	T023	1 2 2 1 2	
1.495E+00	4.219E+02	12.5	T023	1 2 2 1 2	
1.522E+00	4.294E+02	19.9	T023	1 2 2 1 2	
1.566E+00	4.418E+02	27.6	T023	1 2 2 1 2	
1.613E+00	4.550E+02	34.6	T023	1 2 2 1 2	
1.447E+00	4.081E+02	.0	T023	1 2 2 1 2	

654. C_6H_5Cl

Chlorobenzene
IP Carrier T 40
Phenyl chloride
Tetrosin SP
Monochlorobenzene
MCB

RN: 108-90-7 **MP** (°C)**:** −45
MW: 112.56 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-03	4.802E-01	20	K337	1 0 0 0 2	
4.440E-03	4.998E-01	20	M312	1 0 0 0 2	
4.742E-03	5.337E-01	21	C024	2 1 1 2 2	
4.442E-03	5.000E-01	25	A003	1 2 1 2 1	
4.191E-03	4.717E-01	25	A058	1 1 1 1 2	
<1.78E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.460E-03	5.020E-01	25	B304	2 0 2 2 2	
4.300E-03	4.840E-01	25	B317	0 0 0 0 0	
3.108E-03	3.499E-01	25	L319	1 0 2 1 1	
2.620E-03	2.949E-01	25	M342	1 0 1 1 2	
3.540E-02	3.984E+00	25	N309	1 0 0 0 1	*sic*
3.780E-03	4.255E-01	25	S359	2 1 2 2 2	
4.430E-03	4.986E-01	25	W300	2 2 2 2 2	
9.762E-03	1.099E+00	25.50	O005	2 0 2 2 1	*sic*
8.884E-04	1.000E-01	26.70	L095	2 2 1 1 2	
3.980E-03	4.480E-01	30	F071	1 1 2 1 2	
4.353E-03	4.900E-01	30	F300	1 0 0 0 1	
4.333E-03	4.878E-01	30	G029	1 0 2 2 2	
3.980E-03	4.480E-01	30	H080	1 0 0 0 2	
4.000E-03	4.502E-01	30	H332	2 2 2 2 0	
4.351E-03	4.898E-01	30	K065	2 0 2 1 2	
4.211E-03	4.740E-01	30	M300	1 1 2 2 2	
4.211E-03	4.740E-01	30	M311	1 1 2 2 2	
4.298E-03	4.838E-01	30	V009	1 0 0 0 1	
6.259E-03	7.045E-01	40	K065	2 0 2 1 2	
3.560E-03	4.007E-01	45	N043	1 0 2 2 2	
8.521E-03	9.591E-01	50	K065	2 0 2 1 2	
9.762E-03	1.099E+00	60	K065	2 0 2 1 2	
1.424E-02	1.602E+00	70	K065	2 0 2 1 2	
1.601E-02	1.802E+00	80	K065	2 0 2 1 2	
2.216E-02	2.494E+00	90	K065	2 0 2 1 2	
4.185E-03	4.711E-01	ns	H123	0 0 0 0 0	
2.620E-03	2.949E-01	ns	M308	0 0 1 1 2	
4.193E-03	4.720E-01	ns	M344	0 0 0 0 2	

655. $C_6H_5ClN_2O_4S$

4-Chloro-3-nitro-benzenesulfonamide
Benzenesulfonamide, 4-chloro-3-nitro-
RN: 97-09-6 **MP** (°C)**:**
MW: 236.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-04	2.248E-01	15	K024	1 2 1 1 2	

656. C_6H_5ClO

m-Chlorophenol
3-Chlorophenol
Chlorophenate
3-Hydroxychlorobenzene
RN: 108-43-0 **MP** (°C)**:** 33
MW: 128.56 **BP** (°C)**:** 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-01	2.500E+01	20	F300	1 0 0 0 1	
1.919E-01	2.468E+01	20	N034	1 0 0 0 2	
1.726E-01	2.219E+01	25	M373	1 0 2 1 2	
1.995E-01	2.565E+01	ns	R427	0 0 0 0 0	

657. C_6H_5ClO

p-Chlorophenol
4-Chloro-phenol-
Parachlorophenol
4-Hydroxychlorobenze
4-Chlorophenol
4-Hydroxychlorobenzene
RN: 106-48-9 **MP** (°C)**:** 43.2
MW: 128.56 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.815E-01	2.334E+01	15.1	A400	2 1 2 2 2	
2.022E-01	2.600E+01	20	F300	1 0 0 0 1	
1.022E-01	1.314E+01	20	H301	0 0 0 0 0	
1.993E-01	2.563E+01	20	N034	1 0 0 0 2	
1.839E-01	2.364E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.100E-01	2.700E+01	25	B316	0 0 0 0 0	
2.053E-01	2.639E+01	25	M373	1 0 2 1 2	
1.823E-01	2.344E+01	25	R041	0 0 0 0 0	
1.987E-01	2.554E+01	25.2	A400	2 1 2 2 2	
1.867E-01	2.401E+01	34.5	A400	2 1 2 2 2	
4.898E+00	6.297E+02	ns	R427	0 0 0 0 0	

658. C_6H_5ClO

o-Chlorophenol
2-Chlorophenol

RN: 95-57-8 **MP** (°C)**:** 9.3
MW: 128.56 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.621E-01	2.084E+01	15.4	A400	2 1 2 2 2	
1.763E-01	2.266E+01	24.6	A400	2 1 2 2 2	
8.830E-02	1.135E+01	25	B173	2 0 2 2 2	
1.809E-01	2.326E+01	25	M373	1 0 2 1 2	
1.674E-01	2.153E+01	25	R041	0 0 0 0 0	
2.097E-01	2.695E+01	ns	N034	0 0 0 0 2	

659. $C_6H_5ClO_3S$

p-Chlorobenzenesulfonic acid
4-Chlor-benzolsulfosaeure

RN: 98-66-8 **MP** (°C)**:** 67
MW: 192.62 **BP** (°C)**:** 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	4.975E+02	59.0	T023	1 2 2 1 2	
2.590E+00	4.988E+02	62.4	T023	1 2 2 1 2	

660. $C_6H_5ClO_3S.2.5H_2O$

p-Chlorobenzenesulfonic acid (2.5 hydrate)

RN: 98-66-8 **MP** (°C)**:**
MW: 237.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.519E+00	3.609E+02	–26.0	T023	1 2 2 1 2	
1.553E+00	3.690E+02	–20.0	T023	1 2 2 1 2	
1.606E+00	3.816E+02	–11.0	T023	1 2 2 1 2	
1.653E+00	3.929E+02	–2.2	T023	1 2 2 1 2	
1.723E+00	4.095E+02	10.6	T023	1 2 2 1 2	
1.784E+00	4.240E+02	22.9	T023	1 2 2 1 2	
1.817E+00	4.318E+02	27.6	T023	1 2 2 1 2	
1.854E+00	4.406E+02	30.8	T023	1 2 2 1 2	

661. $C_6H_5Cl_2NO_2S$

3,4-Dichloro-benzenesulfonamide
Benzenesulfonamide, 3,4-dichloro-

RN: 23815-28-3 **MP** (°C)**:**
MW: 226.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	7.913E-01	15	K024	1 2 1 1 2	

662. $C_6H_5Cl_2PS$
Dichlorophenylphosphine sulfide
Benzene phosphorus thiodichloride
Phenylphosphonothioic dichloride
Phenyl phosphorus thiodichloride
DCPPS
RN: 3497-00-5 **MP** (°C)**:**
MW: 211.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.211E-03	1.522E+00	23	W402	0 0 0 0 0	
2.597E-02	5.481E+00	32	W402	0 0 0 0 0	
4.676E-02	9.868E+00	40	W402	0 0 0 0 0	
7.060E-02	1.490E+01	50	W402	0 0 0 0 0	

663. C_6H_5F
Fluorobenzene
Fluorbenzol
RN: 462-06-6 **MP** (°C)**:** –42
MW: 96.11 **BP** (°C)**:** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	1.550E+00	25	A003	1 2 1 2 2	
1.602E-02	1.540E+00	30	F071	1 1 2 1 2	
1.561E-02	1.500E+00	30	F300	1 0 0 0 1	
1.602E-02	1.540E+00	30	H080	1 0 0 0 2	
1.600E-02	1.538E+00	30	J036	0 0 0 0 0	
1.598E-02	1.535E+00	30	V009	1 0 0 0 2	
1.616E-02	1.553E+00	ns	M344	0 0 0 0 2	

664. $C_6H_5FN_2O_3$
3-Acetyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Acetyl-5-fluorouracil
RN: 75410-15-0 **MP** (°C)**:** 115–116
MW: 172.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-01	4.280E+01	22	B321	0 0 0 0 0	pH 4.0
1.660E-01	2.857E+01	22	B416	2 2 1 2 1	

665. $C_6H_5FN_2O_4$
1-Methoxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, methyl ester
RN: 71759-43-8 **MP** (°C)**:**
MW: 188.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	2.330E+01	22	B332	1 1 0 0 1	pH 4.0

666. C_6H_5FO

2-Fluorophenol
2-Fluor-phenol
o-Fluorophenol

RN: 367-12-4 **MP** (°C)**:** 16.1
MW: 112.10 **BP** (°C)**:** 171.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

667. C_6H_5FO

m-Fluorophenol
3-Fluorophenol

RN: 372-20-3 **MP** (°C)**:** 13.7
MW: 112.10 **BP** (°C)**:** 178

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	7.735E+01	25	P031	0 0 0 0 0	

668. C_6H_5FO

p-Fluorophenol
4-Fluorophenol

RN: 371-41-5 **MP** (°C)**:** 46–48
MW: 112.10 **BP** (°C)**:** 185–188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.671E-01	6.357E+01	20	R087	0 0 0 0 0	0.15M NaCl
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

669. $C_6H_5FO_3S.H_2O$

p-Fluorobenzenesulfonic acid (monohydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 194.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E+00	4.355E+02	22.1	T023	1 2 2 1 2	
2.263E+00	4.394E+02	35.4	T023	1 2 2 1 2	
2.549E+00	4.950E+02	41.4	T023	1 2 2 1 2	
2.306E+00	4.477E+02	54.2	T023	1 2 2 1 2	
2.539E+00	4.930E+02	54.3	T023	1 2 2 1 2	
2.356E+00	4.575E+02	71.2	T023	1 2 2 1 2	
2.509E+00	4.872E+02	74.5	T023	1 2 2 1 2	
2.392E+00	4.644E+02	80.0	T023	1 2 2 1 2	
2.496E+00	4.847E+02	81.0	T023	1 2 2 1 2	
2.463E+00	4.782E+02	85.2	T023	1 2 2 1 2	
2.440E+00	4.739E+02	85.5	T023	1 2 2 1 2	

670. $C_6H_5FO_3S.2.5H_2O$

p-Fluorobenzenesulfonic acid (2.5 hydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 221.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.848E+00	4.088E+02	–15.5	T023	1 2 2 1 2	
1.880E+00	4.160E+02	–3.9	T023	1 2 2 1 2	
1.893E+00	4.187E+02	1.0	T023	1 2 2 1 2	
1.923E+00	4.254E+02	10.1	T023	1 2 2 1 2	
1.966E+00	4.349E+02	21.3	T023	1 2 2 1 2	

671. $C_6H_5FO_3S.3H_2O$

p-Fluorobenzenesulfonic acid (trihydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 230.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.731E+00	3.985E+02	–22.5	T023	1 2 2 1 2	
1.704E+00	3.922E+02	–21.4	T023	1 2 2 1 2	
1.751E+00	4.032E+02	–19.5	T023	1 2 2 1 2	
1.760E+00	4.052E+02	–17.9	T023	1 2 2 1 2	
1.715E+00	3.949E+02	–18.5	T023	1 2 2 1 2	
1.751E+00	4.032E+02	–13.0	T023	1 2 2 1 2	
1.784E+00	4.108E+02	–7.4	T023	1 2 2 1 2	

672. $C_6H_5FO_3S.4H_2O$

p-Fluorobenzenesulfonic acid (tetrahydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 248.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E+00	3.648E+02	–38.0	T023	1 2 2 1 2	
1.484E+00	3.684E+02	–35.4	T023	1 2 2 1 2	
1.498E+00	3.719E+02	–34.4	T023	1 2 2 1 2	
1.519E+00	3.771E+02	–32.5	T023	1 2 2 1 2	
1.532E+00	3.803E+02	–30.5	T023	1 2 2 1 2	
1.580E+00	3.922E+02	–26.4	T023	1 2 2 1 2	
1.605E+00	3.985E+02	–24.0	T023	1 2 2 1 2	

673. C_6H_5I

Iodobenzene

RN: 591-50-4 **MP** (°C)**:** –30
MW: 204.01 **BP** (°C)**:** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.823E-04	1.800E-01	25	A003	1 2 1 2 1	
9.840E-04	2.007E-01	25	M342	1 0 1 1 2	

(*continued*)

673. C_6H_5I (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-03	3.400E-01	30	F071	1 1 2 1 2	
1.667E-03	3.400E-01	30	F300	1 0 0 0 2	
1.667E-03	3.400E-01	30	H080	1 0 0 0 2	
1.667E-03	3.400E-01	30	M344	1 0 0 0 2	
1.699E-03	3.467E-01	30	V009	1 0 0 0 1	

674. C_6H_5IO

p-Iodophenol
4-Iodophenol

RN: 540-38-5 **MP** (°C)**:** 94
MW: 220.01 **BP** (°C)**:** 138 at 5 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-02	2.828E+00	20	R087	0 0 0 0 0	0.15M NaCl

675. $C_6H_5NO_2$

Nitrobenzene
Nitrobenzol
Benzene, nitro-

RN: 98-95-3 **MP** (°C)**:** 6
MW: 123.11 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	1.700E+00	6	V004	1 0 1 2 2	
1.438E-02	1.770E+00	9.99	B403	1 2 2 2 2	
1.443E-02	1.777E+00	15	G029	1 0 2 2 2	
1.568E-02	1.930E+00	19.99	B403	1 2 2 2 2	
1.549E-02	1.907E+00	20	B179	0 0 0 0 0	
1.543E-02	1.900E+00	20	F300	1 0 0 0 1	
1.600E-02	1.970E+00	20	P073	1 0 0 1 2	
1.543E-02	1.900E+00	22.5	G301	0 0 0 0 0	
1.568E-02	1.930E+00	25	A003	1 2 1 2 2	
1.700E-02	2.093E+00	25	B173	2 0 2 2 2	
1.580E-02	1.945E+00	25	H071	2 2 2 1 2	
1.600E-02	1.970E+00	25	H332	2 2 2 2 1	
1.560E-02	1.921E+00	25	I334	2 2 2 1 2	
1.560E-02	1.921E+00	25	I335	2 2 2 2 2	
1.543E-02	1.900E+00	25	M087	1 1 2 1 2	
1.457E-02	1.794E+00	25.04	V013	2 2 2 2 2	
1.446E-02	1.780E+00	26.70	L095	2 2 1 1 2	
1.673E-02	2.060E+00	29.99	B403	1 2 2 2 2	
1.662E-02	2.046E+00	30	G029	1 0 2 2 2	
1.673E-02	2.060E+00	30	V004	1 0 1 2 2	
1.667E-02	2.052E+00	30	V009	1 0 0 0 2	
1.835E-02	2.259E+00	35	H077	2 2 2 2 2	

(*continued*)

675. $C_6H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-02	2.200E+00	39.99	B403	1 2 2 2 2	
2.144E-02	2.640E+00	50	V004	1 0 1 2 2	
2.193E-02	2.700E+00	55	F300	1 0 0 0 1	
2.534E-02	3.120E+00	60	V004	1 0 1 2 2	
2.700E-03	3.324E-01	ns	D348	0 0 0 0 0	

676. $C_6H_5NO_2$

Nicotinic acid
Niacin

RN: 59-67-6 **MP** (°C)**:** 236
MW: 123.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-01	1.488E+01	1	H083	1 2 2 1 2	
2.679E-01	3.298E+01	16	C033	1 0 2 1 2	
1.358E-01	1.672E+01	20	D041	1 0 0 0 1	
1.436E-01	1.768E+01	20	H083	1 2 2 1 2	
1.381E-01	1.700E+01	20	M054	1 0 0 0 1	
3.652E-01	4.496E+01	28	C033	1 0 2 1 2	
2.595E-01	3.195E+01	42	H083	1 2 2 1 2	
3.735E-01	4.598E+01	60	H083	1 2 2 1 2	
5.604E-01	6.899E+01	80	H083	1 2 2 1 2	
6.809E-01	8.383E+01	88	H083	1 2 2 1 2	

677. $C_6H_5NO_3$

o-Nitrophenol
2-Nitrophenol

RN: 88-75-5 **MP** (°C)**:** 44
MW: 139.11 **BP** (°C)**:** 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.434E-03	8.950E-01	9.99	B403	1 2 2 2 2	
7.735E-03	1.076E+00	15.6	A400	2 1 2 2 2	
9.704E-03	1.350E+00	19.99	B403	1 2 2 2 2	
1.000E-02	1.391E+00	20	H306	1 0 1 2 1	
9.906E-03	1.378E+00	23.10	E032	1 2 1 2 2	
1.220E-02	1.697E+00	24.8	A400	2 1 2 2 2	
1.793E-02	2.494E+00	25	D006	1 2 0 1 2	
1.797E-02	2.500E+00	25	D059	1 2 1 1 1	
1.438E-02	2.000E+00	29.99	B403	1 2 2 2 2	
1.163E-02	1.617E+00	30.40	E032	1 2 1 2 2	
2.110E-02	2.935E+00	34.7	A400	2 1 2 2 2	
1.456E-02	2.026E+00	36.20	E032	1 2 1 2 2	
2.300E-02	3.200E+00	38.40	F300	1 0 0 0 1	
1.936E-02	2.693E+00	39.80	E032	1 2 1 2 2	

(*continued*)

677. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.042E-02	2.840E+00	39.99	B403	1 2 2 2 2	
2.157E-02	3.000E+00	40	D059	1 2 1 1 0	
2.864E-02	3.984E+00	54.60	E032	1 2 1 2 1	
3.598E-02	5.005E+00	67.20	E032	1 2 1 2 2	
4.429E-02	6.162E+00	72.10	E032	1 2 1 2 2	
5.174E-02	7.198E+00	86.90	E032	1 2 1 2 2	
6.560E-02	9.126E+00	93.80	E032	1 2 1 2 2	
7.979E-02	1.110E+01	100	F300	1 0 0 0 2	

678. $C_6H_5NO_3$

p-Nitrophenol
4-Nitrophenol

RN: 100-02-7 **MP** (°C)**:** 113
MW: 139.11 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-02	4.975E+00	0	D006	1 2 0 1 1	
5.787E-02	8.050E+00	9.99	B403	1 2 2 2 2	
7.821E-02	1.088E+01	12.5	D006	1 2 0 1 1	
7.610E-02	1.059E+01	12.60	E032	1 2 1 2 2	
5.780E-02	8.040E+00	15	D069	1 2 0 0 2	
7.305E-02	1.016E+01	15.3	A400	2 1 2 2 2	
1.139E-01	1.584E+01	17.30	E032	1 2 1 2 2	
8.770E-02	1.220E+01	19.99	B403	1 2 2 2 2	
9.700E-02	1.349E+01	20	H306	1 0 1 2 1	
7.188E-02	9.999E+00	20	T301	1 2 2 2 2	
1.078E-01	1.500E+01	22.5	G301	0 0 0 0 0	
1.132E-01	1.575E+01	25	D006	1 2 0 1 1	
1.797E-01	2.500E+01	25	D059	1 2 1 1 1	
8.411E-02	1.170E+01	25	F300	1 0 0 0 2	
9.925E-02	1.381E+01	25	R041	0 0 0 0 0	
1.121E-01	1.560E+01	25.0	A400	2 1 2 2 2	
1.430E-01	1.990E+01	26.60	E032	1 2 1 2 2	
1.794E-01	2.496E+01	27.70	E032	1 2 1 2 2	
2.101E-01	2.922E+01	29.60	E032	1 2 1 2 2	
1.280E-01	1.780E+01	29.99	B403	1 2 2 2 2	
1.409E-01	1.960E+01	30.3	A400	2 1 2 2 2	
1.930E-01	2.685E+01	34.9	A400	2 1 2 2 2	
1.718E-01	2.390E+01	37.99	B403	1 2 2 2 2	
2.026E-01	2.818E+01	40	D006	1 2 0 1 1	
2.085E-01	2.900E+01	40	D059	1 2 1 1 1	
3.021E+00	4.203E+02	40.60	E032	1 2 1 2 2	
2.678E-01	3.726E+01	40.70	E032	1 2 1 2 2	
3.081E+00	4.286E+02	42.50	E032	1 2 1 2 2	
2.961E+00	4.120E+02	42.70	E032	1 2 1 2 2	
3.196E+00	4.447E+02	49.70	E032	1 2 1 2 2	
4.350E-01	6.052E+01	50	D069	1 2 0 0 2	
4.148E-01	5.770E+01	50	F300	1 0 0 0 2	

(*continued*)

678. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.096E-01	4.306E+01	53.30	E032	1 2 1 2 2	
2.900E+00	4.034E+02	54.90	E032	1 2 1 2 2	
3.423E-01	4.762E+01	55.10	E032	1 2 1 2 2	
3.305E+00	4.598E+02	60.70	E032	1 2 1 2 2	
2.834E+00	3.942E+02	65.00	E032	1 2 1 2 2	
3.986E-01	5.545E+01	67.80	E032	1 2 1 2 2	
5.021E-01	6.985E+01	69.40	E032	1 2 1 2 2	
2.768E+00	3.850E+02	73.30	E032	1 2 1 2 2	
3.406E+00	4.739E+02	75.70	E032	1 2 1 2 2	
6.553E-01	9.116E+01	78.30	E032	1 2 1 2 2	
6.837E-01	9.510E+01	79.80	E032	1 2 1 2 2	
2.699E+00	3.754E+02	80.30	E032	1 2 1 2 2	
7.124E-01	9.910E+01	80.70	E032	1 2 1 2 2	
7.987E-01	1.111E+02	82.30	E032	1 2 1 2 2	
9.431E-01	1.312E+02	85.70	E032	1 2 1 2 2	
2.555E+00	3.554E+02	86.00	E032	1 2 1 2 2	
1.076E+00	1.497E+02	88.50	E032	1 2 1 2 2	
2.398E+00	3.336E+02	89.70	E032	1 2 1 2 2	
1.320E+00	1.837E+02	90.70	E032	1 2 1 2 2	
1.438E+00	2.000E+02	91.30	E032	1 2 1 2 2	
2.234E+00	3.107E+02	91.30	E032	1 2 1 2 2	
1.664E+00	2.315E+02	92.10	E032	1 2 1 2 2	
2.056E+00	2.861E+02	92.70	E032	1 2 1 2 2	
1.763E+00	2.453E+02	92.80	E032	1 2 1 2 2	
1.865E+00	2.595E+02	92.90	E032	1 2 1 2 2	
3.503E+00	4.873E+02	93.50	E032	1 2 1 2 2	
5.100E-02	7.095E+00	ns	B157	0 0 0 0 1	
1.148E-01	1.597E+01	ns	R427	0 0 0 0 0	

679. $C_6H_5NO_3$

m-Nitrophenol
3-Nitrophenol

RN: 554-84-7 **MP** (°C)**:** 97
MW: 139.11 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.412E-02	8.920E+00	0	D006	1 2 0 1 1	
5.176E-02	7.200E+00	9.99	B403	1 2 2 2 2	
8.524E-02	1.186E+01	12.5	D006	1 2 0 1 1	
1.243E-01	1.730E+01	15.90	E032	1 2 1 2 2	
7.764E-02	1.080E+01	19.99	B403	1 2 2 2 2	
8.300E-02	1.155E+01	20	H306	1 0 1 2 1	
1.368E-01	1.903E+01	20.20	E032	1 2 1 2 2	
1.458E-01	2.028E+01	23.40	E032	1 2 1 2 2	
9.575E-02	1.332E+01	25	D006	1 2 0 1 2	
9.740E-02	1.355E+01	25	K040	1 0 2 1 2	
9.225E-02	1.283E+01	25	R041	0 0 0 0 0	

(*continued*)

679. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-01	2.344E+01	29.50	E032	1 2 1 2 2	
1.200E-01	1.670E+01	29.99	B403	1 2 2 2 2	
1.366E-01	1.900E+01	34.99	B403	1 2 2 2 2	
1.944E-01	2.705E+01	35.80	E032	1 2 1 2 2	
2.113E-01	2.940E+01	40	F300	1 0 0 0 2	
2.148E-01	2.988E+01	40.90	E032	1 2 1 2 2	
3.196E+00	4.445E+02	47.10	E032	1 2 1 2 2	
3.046E+00	4.237E+02	49.60	E032	1 2 1 2 2	
3.240E+00	4.507E+02	49.70	E032	1 2 1 2 2	
3.313E+00	4.609E+02	56.50	E032	1 2 1 2 2	
2.979E+00	4.145E+02	58.70	E032	1 2 1 2 2	
2.911E-01	4.049E+01	58.80	E032	1 2 1 2 2	
3.475E-01	4.834E+01	62.70	E032	1 2 1 2 2	
3.387E+00	4.712E+02	62.80	E032	1 2 1 2 2	
2.914E+00	4.054E+02	71.50	E032	1 2 1 2 2	
3.484E+00	4.846E+02	75.10	E032	1 2 1 2 2	
4.703E-01	6.542E+01	77.10	E032	1 2 1 2 2	
2.828E+00	3.935E+02	80.60	E032	1 2 1 2 2	
6.326E-01	8.801E+01	85.30	E032	1 2 1 2 2	
3.549E+00	4.937E+02	85.80	E032	1 2 1 2 2	
2.705E+00	3.762E+02	89.40	E032	1 2 1 2 2	
3.569E+00	4.965E+02	89.80	E032	1 2 1 2 2	
2.649E+00	3.684E+02	92.20	E032	1 2 1 2 2	
9.501E-01	1.322E+02	93.60	E032	1 2 1 2 2	
2.581E+00	3.591E+02	94.20	E032	1 2 1 2 2	
2.475E+00	3.443E+02	95.60	E032	1 2 1 2 2	
1.210E+00	1.683E+02	96.20	E032	1 2 1 2 2	
2.396E+00	3.333E+02	96.60	E032	1 2 1 2 2	
1.440E+00	2.004E+02	97.50	E032	1 2 1 2 2	
2.286E+00	3.181E+02	97.70	E032	1 2 1 2 2	
1.604E+00	2.232E+02	98.10	E032	1 2 1 2 2	
2.341E+00	3.256E+02	98.10	E032	1 2 1 2 2	
1.763E+00	2.453E+02	98.40	E032	1 2 1 2 2	
2.049E+00	2.851E+02	98.50	E032	1 2 1 2 2	
1.965E+00	2.734E+02	98.60	E032	1 2 1 2 2	
3.008E+00	4.184E+02	98.70	F300	1 0 0 0 2	
9.772E-02	1.359E+01	ns	R427	0 0 0 0 0	

680. $C_6H_5NO_4$

Nitrohydroquinone
2-Nitroquinol
4-Hydroxy-2-nitrophenol

RN: 16090-33-8 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.888E-02	1.068E+01	30.20	E032	1 2 1 2 2	
1.015E-01	1.575E+01	34.60	E032	1 2 1 2 2	

(*continued*)

680. $C_6H_5NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E-01	2.439E+01	44.60	E032	1 2 1 2 2	
1.999E-01	3.101E+01	49.60	E032	1 2 1 2 2	
3.128E-01	4.853E+01	54.50	E032	1 2 1 2 2	
4.498E-01	6.977E+01	59.10	E032	1 2 1 2 2	
6.405E-01	9.934E+01	61.70	E032	1 2 1 2 2	
7.163E-01	1.111E+02	64.20	E032	1 2 1 2 2	
8.409E-01	1.304E+02	65.00	E032	1 2 1 2 2	
1.074E+00	1.667E+02	93.80	E032	1 2 1 2 2	

681. $C_6H_5NO_4$

4-Nitroresorcinol
4-Nitro-1,3-benzenediol

RN: 3163-07-3 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.354E-02	6.754E+00	18.30	E032	1 2 1 2 2	
5.244E-02	8.133E+00	24.70	E032	1 2 1 2 2	
6.510E-02	1.010E+01	30.80	E032	1 2 1 2 2	
7.959E-02	1.235E+01	36.90	E032	1 2 1 2 2	
1.034E-01	1.604E+01	43.50	E032	1 2 1 2 2	
1.462E-01	2.267E+01	47.50	E032	1 2 1 2 2	
1.817E-01	2.818E+01	49.10	E032	1 2 1 2 2	
2.168E-01	3.363E+01	50.70	E032	1 2 1 2 2	
2.497E-01	3.874E+01	51.20	E032	1 2 1 2 2	
2.776E-01	4.306E+01	52.30	E032	1 2 1 2 2	
3.286E-01	5.096E+01	53.90	E032	1 2 1 2 2	
4.487E-01	6.959E+01	57.80	E032	1 2 1 2 2	
5.951E-01	9.231E+01	62.70	E032	1 2 1 2 2	
8.468E-01	1.313E+02	68.40	E032	1 2 1 2 2	
1.075E+00	1.667E+02	71.90	E032	1 2 1 2 2	
1.209E+00	1.875E+02	72.90	E032	1 2 1 2 2	
1.325E+00	2.055E+02	73.30	E032	1 2 1 2 2	
1.487E+00	2.307E+02	73.40	E032	1 2 1 2 2	

682. $C_6H_5NO_4$

2-Nitroresorcinol
2-Nitro-1,3-benzenediol

RN: 601-89-8 **MP** (°C)**:** 81
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.435E-03	1.308E+00	28.40	E032	1 2 1 2 2	
1.306E-02	2.026E+00	36.70	E032	1 2 1 2 2	
2.319E-02	3.597E+00	47.60	E032	1 2 1 2 2	
3.635E-02	5.638E+00	54.90	E032	1 2 1 2 2	

(*continued*)

682. $C_6H_5NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.276E-02	9.734E+00	67.20	E032	1 2 1 2 2	
8.399E-02	1.303E+01	74.40	E032	1 2 1 2 2	
1.208E-01	1.874E+01	82.90	E032	1 2 1 2 2	
1.529E-01	2.372E+01	92.30	E032	1 2 1 2 2	

683. $C_6H_5NO_4$

3-Nitrocatechol
3-Nitro-1,2-benzenediol
RN: 6665-98-1 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.377E-02	8.340E+00	14.40	E032	1 2 1 2 2	
6.573E-02	1.019E+01	20.90	E032	1 2 1 2 2	
9.590E-02	1.488E+01	29.50	E032	1 2 1 2 2	
1.277E-01	1.980E+01	35.10	E032	1 2 1 2 2	
1.474E-01	2.286E+01	37.90	E032	1 2 1 2 2	
1.738E-01	2.695E+01	41.00	E032	1 2 1 2 2	
2.372E-01	3.679E+01	45.80	E032	1 2 1 2 2	
2.646E-01	4.104E+01	47.60	E032	1 2 1 2 2	
3.216E-01	4.988E+01	54.50	E032	1 2 1 2 2	
3.615E-01	5.607E+01	61.30	E032	1 2 1 2 2	
4.548E-01	7.055E+01	75.90	E032	1 2 1 2 2	
5.743E-01	8.909E+01	86.80	E032	1 2 1 2 2	
8.164E-01	1.266E+02	96.80	E032	1 2 1 2 2	

684. $C_6H_5NO_4$

4-Nitrocatechol
4-Nitro-1,2-benzenediol
RN: 3316-09-4 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E+00	1.878E+02	24.60	E032	1 2 1 2 2	
1.423E+00	2.208E+02	37.70	E032	1 2 1 2 2	
1.488E+00	2.308E+02	41.30	E032	1 2 1 2 2	
1.664E+00	2.582E+02	51.90	E032	1 2 1 2 2	
1.829E+00	2.837E+02	58.50	E032	1 2 1 2 2	
2.004E+00	3.109E+02	66.50	E032	1 2 1 2 2	
2.049E+00	3.179E+02	67.80	E032	1 2 1 2 2	
2.149E+00	3.334E+02	71.20	E032	1 2 1 2 2	

685. $C_6H_5NO_5S$

p-Nitrobenzenesulfonic acid
4-Nitrobenzenesulfonic acid
RN: 138-42-1 **MP** (°C)**:**
MW: 203.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E+00	4.760E+02	100.5	T023	1 2 2 1 2	
2.412E+00	4.901E+02	105.0	T023	1 2 2 1 2	
2.461E+00	5.000E+02	110.0	T023	1 2 2 1 2	

686. $C_6H_5NO_5S.2H_2O$

p-Nitrobenzenesulfonic acid (dihydrate)
RN: 15481-55-7 **MP** (°C)**:**
MW: 239.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E+00	3.987E+02	36.6	T023	1 2 2 1 2	
1.720E+00	4.113E+02	56.6	T023	1 2 2 1 2	
1.771E+00	4.235E+02	75.5	T023	1 2 2 1 2	
1.822E+00	4.359E+02	90.2	T023	1 2 2 1 2	
1.939E+00	4.638E+02	106.8	T023	1 2 2 1 2	
1.920E+00	4.592E+02	110.2	T023	1 2 2 1 2	

687. $C_6H_5NO_5S.4H_2O$

p-Nitrobenzenesulfonic acid (tetrahydrate)
RN: 15481-55-7 **MP** (°C)**:**
MW: 275.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E+00	2.919E+02	–8.3	T023	1 2 2 1 2	
1.146E+00	3.153E+02	–1.0	T023	1 2 2 1 2	
1.273E+00	3.504E+02	10.8	T023	1 2 2 1 2	
1.318E+00	3.627E+02	16.0	T023	1 2 2 1 2	
1.409E+00	3.877E+02	26.3	T023	1 2 2 1 2	

688. $C_6H_5N_2OS$

Methyl acetylthiodiazole
Thiodiazolique methyle acetyle
RN: **MP** (°C)**:**
MW: 153.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.528E-04	1.000E-01	37	D084	1 0 1 0 1	

689. $C_6H_5N_3$
Benzotriazole
1,2,3-Benzotriazole
Cobratec 99
1,2,3-triaza-1H-indene
Azimidobenzene
Benzene azimide
RN: 95-14-7 **MP** (°C)**:** 98.5
MW: 119.13 **BP** (°C)**:** 350

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-01	1.977E+01	ns	R427	0 0 0 0 0	

690. $C_6H_5N_3O_4$
2,6-Dinitroaniline
2,6-Dinitrobenzenamine
RN: 606-22-4 **MP** (°C)**:** 133
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	7.994E-02	25	B335	1 2 0 0 1	

691. $C_6H_5N_3O_4$
2,4-Dinitroaniline
2,4-Dinitrobenzenamine
2,4-Dinitroaminobenzene
1-Amino-2,4-dinitrobenzene
RN: 97-02-9 **MP** (°C)**:** 176
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-04	7.812E-02	25	B335	1 2 0 0 1	

692. $C_6H_5N_3O_5$
Picramic acid
2-Amino-4,6-dinitro-phenol
RN: 96-91-3 **MP** (°C)**:** 169
MW: 199.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-03	1.400E+00	22	F300	1 0 0 0 1	

693. $C_6H_5N_5$
7-Aminopteridine
7-Pteridinamine
RN: 769-66-4 **MP** (°C)**:**
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	20	A083	1 2 0 0 0	
3.974E-02	5.848E+00	100	A083	1 2 0 0 0	

694. $C_6H_5N_5$
4-Aminopteridine
4-Pteridinamine
RN: 6973-01-9 **MP** (°C)**:** 305
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	22.5	A085	1 2 0 0 0	

695. $C_6H_5N_5$
2-Aminopteridine
2-Pteridinamine
RN: 700-81-2 **MP** (°C)**:**
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.031E-03	7.402E-01	22.5	A085	1 2 0 0 0	

696. $C_6H_5N_5O$
4-Amino-2-hydroxypteridine
4-Amino-2-oxopteridine
4-Aminopteridin-2-one
4-Amino-2-pteridone
RN: 22005-65-8 **MP** (°C)**:** >350
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.378E-04	7.142E-02	20	A019	2 2 1 1 2	
5.104E-03	8.326E-01	100	A019	1 2 1 1 2	

697. $C_6H_5N_5O$
2-Amino-4-hydroxypteridine
2-Amino-4(1H)-pteridinone
2-Amino-4(3H)-pteridinone
2-Amino-4-pteridone
2-Amino-4-oxopteridine
2-Aminopteridin-4-one
RN: 2236-60-4 **MP** (°C)**:**
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.075E-04	1.754E-02	22.5	A085	1 2 0 0 0	

698. $C_6H_5N_5O$
7-Amino-6-hydroxypteridine
7-Amino-6-oxopteridine
7-Aminopteridin-6-one
7-Amino-6-pteridone
RN: 1008-85-1 **MP** (°C)**:**
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	2.000E-01	100	A082	1 2 0 0 0	

699. $C_6H_5N_5O_2$
Xanthopterin
2-Amino-4:6-dihydroxypteridine
RN: 119-44-8 **MP** (°C)**:**
MW: 179.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.396E-04	2.500E-02	22.5	A085	1 2 0 0 0	

700. $C_6H_5N_5O_3$
Leucopterin
2-Amino-4:6:7-trihydroxypteridine
RN: 492-11-5 **MP** (°C)**:**
MW: 195.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.833E-06	1.333E-03	22.5	A085	1 2 0 0 0	

701. $C_6H_5N_5O_4S$
3′-Nitrosoniridazole
2-Imidazolidinone, 1-nitroso-3-(5-nitro-2-thiazolyl)-
RN: 34968-90-6 **MP** (°C)**:** 202-203
MW: 243.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.084E-04	7.500E-02	25	G051	1 0 1 1 0	

702. C_6H_6
Benzene
Benzol
Phenyl hydride
Cyclohexatriene
Benzolene
Phene
RN: 71-43-2 **MP** (°C)**:** 5
MW: 78.11 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E-02	1.836E+00	.20	M151	2 1 2 2 2	
2.347E-02	1.833E+00	.24	M183	1 2 1 1 2	
1.959E-02	1.530E+00	0	F300	1 0 0 0 2	
2.148E-02	1.678E+00	0	P003	2 2 2 2 2	
2.356E-02	1.840E+00	.80	A004	1 2 2 1 2	
2.351E-02	1.837E+00	4.50	B086	2 1 2 2 2	
1.881E-02	1.469E+00	4.62	U013	1 0 0 0 0	EFG
2.646E-02	2.067E+00	4.8	L007	2 1 1 2 2	
1.178E-02	9.200E-01	5	S119	0 0 0 0 1	
2.646E-02	2.067E+00	5.0	L007	2 1 1 1 2	
1.838E-02	1.436E+00	5.39	U010	1 0 0 1 1	EFG
2.310E-02	1.804E+00	6.20	M151	2 1 2 2 2	
2.306E-02	1.802E+00	6.24	M183	1 2 1 1 2	
2.364E-02	1.847E+00	6.30	B086	2 1 2 2 2	
2.313E-02	1.807E+00	7.10	B086	2 1 2 2 2	
2.313E-02	1.807E+00	9	B086	2 1 2 2 2	
2.292E-02	1.790E+00	9.40	A004	1 2 2 1 2	
2.080E-02	1.625E+00	10	B149	2 1 1 2 2	
2.110E-02	1.648E+00	10	J302	2 1 2 2 2	
2.240E-02	1.750E+00	10	M130	1 0 0 0 2	
2.300E-02	1.797E+00	11.00	M151	2 1 2 2 2	
2.300E-02	1.796E+00	11.04	M183	1 2 1 1 2	
2.262E-02	1.767E+00	11.80	B086	2 1 2 2 2	
2.262E-02	1.767E+00	12.10	B086	2 1 2 2 2	
2.270E-02	1.773E+00	14.00	M151	2 1 2 2 2	
2.263E-02	1.767E+00	14.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	14.20	U013	1 0 0 0 0	EFG
2.655E-02	2.074E+00	14.8	L007	2 1 1 2 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.655E-02	2.074E+00	14.9	L007	2 1 1 1 2	
2.290E-02	1.789E+00	15	I333	1 2 1 1 2	
2.150E-02	1.679E+00	15	S006	1 0 0 0 2	
1.971E-02	1.540E+00	15	S203	1 1 2 1 2	
1.797E-02	1.403E+00	15.02	U010	1 0 0 1 1	EFG
2.287E-02	1.787E+00	15.10	B086	2 1 2 2 2	
2.112E-02	1.650E+00	16	D047	1 0 0 1 2	
2.266E-02	1.770E+00	16.80	A004	1 2 2 1 2	
2.260E-02	1.765E+00	16.90	M151	2 1 2 2 2	
2.253E-02	1.760E+00	16.94	M183	1 2 1 1 2	
2.191E-02	1.711E+00	17	F002	2 2 2 2 2	
2.287E-02	1.787E+00	17.90	B086	2 1 2 2 2	
2.260E-02	1.765E+00	18.60	M151	2 1 2 2 2	
2.259E-02	1.764E+00	18.64	M183	1 2 1 1 2	
2.664E-02	2.081E+00	19.8	L007	2 1 1 2 2	
2.664E-02	2.081E+00	19.9	L007	2 1 1 1 2	
2.220E-02	1.734E+00	20	B149	2 1 1 2 2	
2.180E-02	1.703E+00	20	C006	1 2 1 1 2	
1.023E-02	7.994E-01	20	C121	0 0 0 0 0	unit assumed, *sic*
2.428E-02	1.896E+00	20	D052	1 1 0 0 1	
1.600E-02	1.250E+00	20	E009	1 0 0 0 1	
1.680E-02	1.312E+00	20	E025	1 0 2 2 2	
2.189E-02	1.710E+00	20	F071	1 1 2 1 2	
2.317E-02	1.810E+00	20	F300	1 0 0 0 2	
1.023E-02	7.994E-01	20	I310	0 0 0 0 0	
2.310E-02	1.804E+00	20	I333	1 2 1 1 2	
2.042E-02	1.595E+00	20	K337	1 0 0 0 2	
2.280E-02	1.781E+00	20	M312	1 0 0 0 1	
1.366E-02	1.067E+00	20	M337	2 1 2 2 2	
2.650E-02	2.070E+00	20	P073	1 0 0 1 2	
1.751E-02	1.368E+00	20.0	H043	2 2 2 2 2	
2.249E-02	1.757E+00	20.10	B086	2 1 2 2 2	
2.224E-02	1.737E+00	21	C024	2 1 1 2 2	
2.202E-02	1.720E+00	22	F002	2 2 2 2 2	
2.320E-02	1.812E+00	22.5	I333	1 2 1 1 2	
2.304E-02	1.800E+00	24	A004	1 2 2 1 2	
2.667E-02	2.084E+00	24.8	L007	2 1 1 2 2	
2.227E-02	1.740E+00	25	A001	1 2 2 2 2	
1.917E-02	1.498E+00	25	A037	2 2 2 2 2	
2.292E-02	1.790E+00	25	B003	2 2 2 2 2	
2.045E-02	1.597E+00	25	B019	1 0 1 2 0	
2.279E-02	1.780E+00	25	B060	2 0 1 1 1	
2.292E-02	1.790E+00	25	B090	2 2 2 1 2	
2.292E-02	1.790E+00	25	B151	1 2 2 1 2	
2.330E-02	1.820E+00	25	B153	2 1 1 1 2	
2.240E-02	1.750E+00	25	B173	2 0 2 2 2	
2.300E-02	1.797E+00	25	G323	2 2 2 2 2	
2.300E-02	1.797E+00	25	H332	2 2 2 2 1	
2.330E-02	1.820E+00	25	I333	1 2 1 1 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-02	1.804E+00	25	J302	2 1 2 2 2	
2.390E-02	1.867E+00	25	K001	2 2 2 2 2	
8.961E-03	7.000E-01	25	K072	1 0 1 1 1	
1.300E-02	1.015E+00	25	K123	1 0 2 2 1	
2.170E-02	1.695E+00	25	K316	2 2 2 2 2	
2.259E-02	1.765E+00	25	L002	2 2 2 2 2	
2.313E-02	1.807E+00	25	L319	1 0 2 1 1	
2.166E-02	1.692E+00	25	L322	1 1 2 2 1	
1.770E+00	1.383E+02	25	M021	2 2 2 1 2	*sic*
2.279E-02	1.780E+00	25	M131	1 0 0 0 2	
2.278E-02	1.780E+00	25	M132	2 2 2 1 2	
2.310E-02	1.804E+00	25	M151	2 1 2 2 2	average of 2
2.293E-02	1.791E+00	25	M151	2 1 1 2 2	
2.290E-02	1.789E+00	25	M342	1 0 1 1 2	
1.917E-02	1.498E+00	25	O015	0 0 0 0 0	
2.247E-02	1.755E+00	25	P003	2 2 2 2 2	
2.227E-02	1.740E+00	25	P051	2 1 1 2 2	
2.607E-02	2.036E+00	25	S010	2 1 2 1 2	
2.377E-02	1.857E+00	25	S012	2 0 2 2 2	
2.061E-02	1.610E+00	25	S203	1 1 2 1 2	
2.070E-02	1.617E+00	25	S359	2 1 2 2 2	
2.778E-02	2.170E+00	25	W057	2 0 2 2 2	
2.290E-02	1.789E+00	25	W300	2 2 2 2 2	
2.300E-02	1.797E+00	25.0	H043	2 2 2 2 2	
2.667E-02	2.084E+00	25.0	L007	2 1 1 1 2	
2.227E-02	1.740E+00	25.00	P007	2 1 2 2 2	
2.290E-02	1.789E+00	25.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	25.35	U010	1 0 0 1 1	EFG
1.881E-02	1.469E+00	25.35	U013	1 0 0 0 0	EFG
2.325E-02	1.816E+00	25.84	M183	1 2 1 1 2	
2.213E-02	1.729E+00	26	F002	2 2 2 2 2	
2.229E-02	1.742E+00	29	F002	2 2 2 2 2	
2.351E-02	1.837E+00	29.99	C349	0 0 0 0 0	
2.368E-02	1.850E+00	30	F300	1 0 0 0 2	
2.364E-02	1.847E+00	30	G029	1 0 2 2 2	
2.350E-02	1.836E+00	30	I333	1 2 1 1 2	
2.343E-02	1.830E+00	31	A004	1 2 2 1 2	
2.285E-02	1.785E+00	32	F002	2 2 2 2 2	
1.970E-02	1.539E+00	34.53	U013	1 0 0 0 0	EFG
2.685E-02	2.098E+00	34.8	L007	2 1 1 2 2	
2.329E-02	1.819E+00	35	F002	2 2 2 2 2	
2.253E-02	1.760E+00	35	S203	1 1 2 1 2	
2.685E-02	2.098E+00	35.1	L007	2 1 1 1 2	
1.925E-02	1.504E+00	35.48	U010	1 0 0 1 1	EFG
2.458E-02	1.920E+00	38	A004	1 2 2 1 2	
2.573E-02	2.010E+00	39.99	C349	0 0 0 0 0	
2.592E-02	2.025E+00	40	B151	1 2 1 1 2	
2.434E-02	1.902E+00	41	F002	2 2 2 2 2	
2.440E-02	1.906E+00	42	F002	2 2 2 2 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.467E-02	1.927E+00	44	F002	2 2 2 2 2	
2.016E-02	1.574E+00	44.30	U010	1 0 0 1 1	EFG
2.062E-02	1.611E+00	44.30	U013	1 0 0 0 0	EFG
2.599E-02	2.030E+00	44.70	A004	1 2 2 1 2	
2.368E-02	1.850E+00	45	S203	1 1 2 1 2	
2.938E-02	2.295E+00	45.7	L007	2 1 1 1 2	
2.938E-02	2.295E+00	45.8	L007	2 1 1 2 2	
2.534E-02	1.979E+00	46	F002	2 2 2 2 2	
2.827E-02	2.208E+00	49.99	C349	0 0 0 0 0	
2.810E-02	2.195E+00	50	G323	2 2 2 2 1	
2.650E-02	2.070E+00	51	F002	2 2 2 2 2	
2.740E-02	2.140E+00	51.50	A004	1 2 2 1 2	
2.159E-02	1.687E+00	53.64	U010	1 0 0 1 1	EFG
2.210E-02	1.726E+00	54.71	U013	1 0 0 0 0	EFG
5.095E-02	3.980E+00	55.3	P051	2 1 1 2 2	
5.095E-02	3.980E+00	55.30	P007	2 1 2 2 2	
2.788E-02	2.178E+00	56	F002	2 2 2 2 2	
3.162E-02	2.470E+00	57	B124	2 2 2 1 2	
3.776E-02	2.950E+00	57.70	B124	1 2 2 1 2	
2.996E-02	2.340E+00	58.80	A004	1 2 2 1 2	
3.131E-02	2.446E+00	59.99	C349	0 0 0 0 0	
2.938E-02	2.295E+00	60	B126	1 0 1 1 1	
3.101E-02	2.422E+00	60	B151	1 2 1 1 2	
2.943E-02	2.299E+00	61	F002	2 2 2 2 2	
3.004E-02	2.347E+00	63	F002	2 2 2 2 2	
3.290E-02	2.570E+00	65.40	A004	1 2 2 1 2	
2.479E-02	1.936E+00	65.82	U013	1 0 0 0 0	EFG
3.597E-02	2.810E+00	69.20	B124	1 2 2 1 2	
3.587E-02	2.802E+00	69.30	B124	1 0 2 2 2	
3.463E-02	2.705E+00	69.99	C349	0 0 0 0 0	
8.280E-02	6.468E+00	74.7	P051	2 1 1 2 2	
8.280E-02	6.468E+00	74.70	P007	2 1 2 2 2	
3.872E-02	3.024E+00	79.99	C349	0 0 0 0 0	
4.429E-02	3.460E+00	89.99	C349	0 0 0 0 0	
2.560E-02	2.000E+00	100	J023	1 1 2 2 0	
5.256E-02	4.106E+00	99.99	C349	0 0 0 0 0	
7.681E-02	6.000E+00	150	J023	1 1 2 2 0	
2.688E-01	2.100E+01	200	J023	1 1 2 2 1	
9.345E-01	7.300E+01	250	J023	1 1 2 2 1	
1.357E+00	1.060E+02	285	J023	1 1 2 2 2	
1.869E+00	1.460E+02	300	J023	1 1 2 2 2	
2.200E-02	1.719E+00	ns	B059	0 0 1 1 2	
4.000E-03	3.125E-01	ns	D348	0 0 0 0 0	
2.279E-02	1.780E+00	ns	H123	0 0 0 0 0	
3.020E-01	2.359E+01	ns	H307	0 0 0 0 0	
4.500E-02	3.515E+00	ns	H333	0 1 0 1 0	EFG
2.330E-02	1.820E+00	ns	I332	0 0 0 0 2	
2.292E-02	1.790E+00	ns	K304	0 0 0 0 2	
1.933E-02	1.510E+00	ns	M010	0 0 0 0 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-02	1.769E+00	ns	M175	0 0 2 1 2	
2.279E-02	1.780E+00	ns	M344	0 0 0 0 2	

703. $C_6H_6BrNO_2S$

4-Bromobenzenesulfonamide
(4-Bromophenyl)sulfonamide
p-Bromobenzenesulfonamide
4-Aminosulfonyl-1-bromobenzene
RN: 701-34-8 **MP** (°C)**:**
MW: 236.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	9.916E-01	15	K024	1 2 1 1 2	

704. $C_6H_6BrNO_3S$

p-Bromoaniline-*o*-sulfonic acid
2-Amino-5-bromophenylsulfonic acid
RN: 1576-59-6 **MP** (°C)**:**
MW: 252.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.107E-02	2.790E+00	8.35	P038	1 0 1 0 2	anhydrate
1.424E-02	3.590E+00	16.75	P038	1 0 1 0 2	anhydrate
1.769E-02	4.460E+00	25.0	P038	1 0 1 0 2	anhydrate
2.578E-02	6.500E+00	40.0	P038	1 0 1 0 2	anhydrate
3.828E-02	9.650E+00	55.0	P038	1 0 1 0 2	anhydrate
5.454E-02	1.375E+01	70.0	P038	1 0 1 0 2	anhydrate
8.013E-02	2.020E+01	85.0	P038	1 0 1 0 2	anhydrate
8.846E-03	2.230E+00	.0	P038	1 0 1 0 2	anhydrate

705. $C_6H_6BrNO_3S$

p-Bromoaniline-*m*-sulfonic acid
5-Amino-2-bromobenzenesulfonic acid
RN: 150454-14-1 **MP** (°C)**:**
MW: 252.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E-02	8.850E+00	9.8	P038	1 2 2 2 2	anhydrous rhombic
2.559E-02	6.450E+00	12.55	P038	1 2 2 2 2	anhydrous monoclinic
4.284E-02	1.080E+01	20.0	P038	1 2 2 2 2	anhydrous rhombic
3.419E-02	8.620E+00	25.0	P038	1 2 2 2 2	anhydrous monoclinic
4.740E-02	1.195E+01	25.0	P038	1 2 2 2 2	anhydrous rhombic
5.177E-02	1.305E+01	29.6	P038	1 2 2 2 2	anhydrous rhombic
5.732E-02	1.445E+01	34.7	P038	1 2 2 2 2	anhydrous rhombic
4.820E-02	1.215E+01	40.0	P038	1 2 2 2 2	anhydrous monoclinic

(*continued*)

705. $C_6H_6BrNO_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.387E-02	1.610E+01	40.1	P038	1 2 2 2 2	anhydrous rhombic
6.922E-02	1.745E+01	44.5	P038	1 2 2 2 2	anhydrous rhombic
7.577E-02	1.910E+01	49.7	P038	1 2 2 2 2	anhydrous rhombic
8.330E-02	2.100E+01	54.8	P038	1 2 2 2 2	anhydrous rhombic
7.101E-02	1.790E+01	56.3	P038	1 2 2 2 2	anhydrous monoclinic
9.600E-02	2.420E+01	62.3	P038	1 2 2 2 2	anhydrous rhombic
9.679E-02	2.440E+01	70.0	P038	1 2 2 2 2	anhydrous monoclinic
1.115E-01	2.810E+01	70.4	P038	1 2 2 2 2	anhydrous rhombic
1.329E-01	3.350E+01	85.0	P038	1 2 2 2 2	anhydrous monoclinic
1.452E-01	3.660E+01	85.0	P038	1 2 2 2 2	anhydrous rhombic
2.880E-02	7.260E+00	.0	P038	1 2 2 2 2	anhydrous rhombic
1.884E-02	4.750E+00	.0	P038	1 2 2 2 2	anhydrous monoclinic

706. $C_6H_6BrNO_3S.H_2O$

p-Bromoaniline-*o*-sulfonic acid (monohydrate)
2-Amino-5-bromophenylsulfonic acid (monohydrate)
RN: 1576-59-6 **MP** (°C)**:**
MW: 270.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.520E+00	8.35	P038	1 0 1 0 2	monohydrate
1.751E-02	4.730E+00	16.8	P038	1 0 1 0 2	monohydrate
2.244E-02	6.060E+00	25.0	P038	1 0 1 0 2	monohydrate
9.589E-03	2.590E+00	.0	P038	1 0 1 0 2	monohydrate

707. C_6H_6ClN

p-Chloroaniline
4-Chloroaniline
RN: 106-47-8 **MP** (°C)**:** 72.5
MW: 127.57 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.157E-02	2.752E+00	20	H118	1 1 1 1 2	
2.157E-02	2.752E+00	20	H301	0 0 0 0 0	
3.057E-02	3.900E+00	22.5	G301	0 0 0 0 0	

708. C_6H_6ClN

o-Chloroaniline
2-Chloroaniline
RN: 95-51-2 **MP** (°C)**:** –1
MW: 127.57 **BP** (°C)**:** 208.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-02	3.765E+00	20	C113	1 0 2 1 2	

709. C_6H_6ClN
m-Chloroaniline
3-Chloroaniline
RN: 108-42-9 **MP** (°C)**:** –10
MW: 127.57 **BP** (°C)**:** 230.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-02	5.442E+00	20	C113	1 0 2 1 2	

710. $C_6H_6ClNO_2S$
m-Chlorobenzenesulfonamide
MON 5783
RN: 17260-71-8 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	6.707E-01	15	K024	1 2 1 1 2	

711. $C_6H_6ClNO_2S$
o-Chlorobenzenesulfonamide
2-Chlorobenzenesulfonamide
RN: 6961-82-6 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.983E-01	15	K024	1 2 1 1 2	

712. $C_6H_6ClNO_2S$
4-Chlorobenzenesulfonamide
p-Chlorobenzenesulfonamide
RN: 98-64-6 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.322E+00	15	K024	1 2 1 1 2	

713. $C_6H_6ClNO_3S$
p-Chloroaniline-*m*-sulfonic acid
1-Amino-4-chlorobenzene-3-sulfonic acid
4-Chloro-3-sulfoaniline
3-Amino-6-chlorobenzenesulfonic acid
RN: 88-43-7 **MP** (°C)**:**
MW: 207.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.447E-02	1.131E+01	0	P038	1 0 1 1 2	anhydrate

714. $C_6H_6ClNO_3S.H_2O$

p-Chloroaniline-*o*-sulfonic acid (monohydrate)
1-Amino-4-chloro-2-benzenesulfonic acid (monohydrate)
RN: 133-74-4 **MP** (°C)**:**
MW: 225.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.387E-02	3.130E+00	0	P038	1 2 2 1 2	monohydrate

715. $C_6H_6ClNO_3S.H_2O$

p-Chloroaniline-*m*-sulfonic acid (monohydrate)
1-Amino-4-chlorobenzene-3-sulfonic acid (monohydrate)
RN: 88-43-7 **MP** (°C)**:**
MW: 225.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.141E-02	1.160E+01	0	P038	1 0 1 1 2	metastable monohydrate

716. $C_6H_6Cl_6$

β-1,2,3,4,5,6-Hexachlorocyclohexane
β-Benzene hexachloride
β-BHC
β-Hexachlorocyclohexane
RN: 319-85-7 **MP** (°C)**:** 312
MW: 290.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-05	5.000E-03	20	C099	1 2 0 0 0	
8.252E-07	2.400E-04	25	W025	1 0 2 2 2	
5.501E-07	1.600E-04	28	K120	1 2 2 2 1	average of 2
1.719E-06	5.000E-04	ns	M061	0 0 0 0 0	

717. $C_6H_6Cl_6$

δ-1,2,3,4,5,6-Hexachlorocyclohexane
δ-Benzene hexachloride
RN: 608-73-1 **MP** (°C)**:**
MW: 290.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
1.080E-04	3.140E-02	25	W025	1 0 2 2 2	
4.009E-05	1.166E-02	28	K120	1 2 2 2 2	average of 4

718. $C_6H_6Cl_6$

Lindane
γ-BHC
Benzene hexachloride

RN: 58-89-9 **MP** (°C)**:** 112.5
MW: 290.83 **BP** (°C)**:** 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.393E-06	2.150E-03	15	B083	2 2 1 2 2	
7.393E-06	2.150E-03	15	B162	1 0 0 0 2	
2.816E-05	8.190E-03	19	I018	1 0 0 0 2	
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
2.709E-05	7.880E-03	22	K137	1 1 2 1 0	
2.706E-05	7.870E-03	24	C313	0 0 0 0 0	
5.845E-05	1.700E-02	24	H116	2 1 0 0 2	
2.338E-05	6.800E-03	25	B083	2 2 1 2 2	
2.338E-05	6.800E-03	25	B162	1 0 0 0 2	
2.586E-05	7.520E-03	25	M060	2 2 1 2 2	
2.510E-05	7.300E-03	25	M130	1 0 0 0 1	
2.682E-05	7.800E-03	25	W025	1 0 2 2 2	
4.126E-05	1.200E-02	27	B161	2 1 2 2 0	EFG
2.235E-05	6.500E-03	28	K120	1 2 2 2 2	average of 4
3.920E-05	1.140E-02	35	B083	2 2 1 2 2	particle size 5 µm
7.221E-05	2.100E-02	35	B161	2 1 2 2 0	EFG
3.920E-05	1.140E-02	35	B162	1 0 0 0 2	
5.226E-05	1.520E-02	45	B083	2 2 1 2 2	particle size 5 µm
9.284E-05	2.700E-02	45	B161	2 1 2 2 0	EFG
1.135E-04	3.300E-02	50	B161	2 1 2 2 0	EFG
1.547E-04	4.500E-02	60	B161	2 1 2 2 0	EFG
2.400E-05	6.980E-03	ns	C318	0 0 0 0 0	
~3.44E-05	~1.00E-02	ns	I308	0 0 0 0 0	
5.158E-07	1.500E-04	ns	K138	0 0 0 0 2	*sic*
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	
2.407E-05	7.000E-03	ns	M110	0 0 0 0 0	EFG
2.510E-05	7.300E-03	ns	V414	0 0 0 0 0	
3.438E-05	1.000E-02	rt	M161	0 0 0 0 1	

719. $C_6H_6Cl_6$

α-1,2,3,4,5,6-Hexachlorocyclohexane
α-Benzene hexachloride
α-HCH
α-BHC
α-Hexachlorocyclohexane

RN: 319-84-6 **MP** (°C)**:** 158
MW: 290.83 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
6.877E-06	2.000E-03	25	W025	1 0 2 2 2	
5.570E-06	1.620E-03	28	K120	1 2 2 2 2	average of 4
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	

720. $C_6H_6FN_3O_3$
1-Methylcarbamoyl-5-fluorouracil
5-Fluoro-3,4-dihydro-*N*-methyl-2,4-dioxo-pyrimidinecarboxamide
1-Methylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
RN: 56563-18-9 **MP** (°C)**:** 225–228
MW: 187.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	6.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.313E-03	6.200E-01	22	B388	0 0 0 0 0	

721. $C_6H_6INO_3S$
2-Iodoaniline-4-sulphonic acid
Benzenesulfonic acid, 4-amino-2-iodo-
RN: 67877-88-7 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.781E-02	2.028E+01	25	B107	1 2 1 1 2	

722. $C_6H_6INO_3S$
3-Iodoaniline-4-sulphonic acid
Benzenesulfonic acid, 4-amino-3-iodo-
RN: 25210-30-4 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-03	1.936E+00	25	B107	1 2 1 1 2	

723. $C_6H_6INO_3S$
4-Iodoaniline-2-sulphonic acid
Benzenesulfonic acid, 2-amino-4-iodo-
RN: 171664-62-3 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.697E-02	5.074E+00	25	B107	1 2 1 1 1	

724. $C_6H_6INO_3S$
4-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-4-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.486E-02	1.342E+01	25	B107	1 2 1 1 2	

725. $C_6H_6INO_3S$
5-Iodoaniline-2-sulphonic acid
Benzenesulfonic acid, 2-amino-5-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.671E-03	2.593E+00	25	B107	1 2 1 1 1	

726. $C_6H_6INO_3S$
6-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-6-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.597E-02	4.777E+00	25	B107	1 2 1 1 1	

727. $C_6H_6INO_3S$
5-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-5-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-02	1.293E+01	25	B107	1 2 1 1 2	

728. $C_6H_6N_2O$
Nicotiamide
Niacinamide
Nicotinamide
RN: 98-92-0 **MP** (°C)**:** 131
MW: 122.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.094E+00	5.000E+02	20	D041	1 0 0 0 2	
8.188E+00	1.000E+03	20	M054	1 0 0 0 2	
2.900E-03	3.542E-01	25	A350	0 0 0 0 0	
8.188E+00	1.000E+03	25	D315	0 0 0 0 0	
8.188E-01	1.000E+02	ns	K444	0 0 0 0 0	

729. $C_6H_6N_2O_2$
3-Nitroaniline
1-Amino-3-nitrobenzene
3-Nitrobenzenamine
m-Nitroaminobenzene
m-Nitroaniline
3-Nitro-anilin
RN: 99-09-2 **MP** (°C)**:** 114
MW: 138.13 **BP** (°C)**:** 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-03	1.203E+00	20	B179	0 0 0 0 0	
5.370E-03	7.418E-01	25	B335	1 2 0 0 1	
6.516E-03	9.000E-01	25	F300	1 0 0 0 2	
3.020E-03	4.171E-01	25	L016	1 0 0 0 2	unit assumed
6.582E-03	9.092E-01	25.0	C026	0 0 0 0 0	
1.290E-02	1.782E+00	40.1	C026	0 0 0 0 0	

730. $C_6H_6N_2O_2$
Urocanic acid
Urocaninsaeure
RN: 104-98-3 **MP** (°C)**:** 225
MW: 138.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E-02	1.500E+00	17.40	F300	1 0 0 0 1	
4.318E-02	5.964E+00	37	D041	1 0 0 0 0	
5.575E-02	7.700E+00	50	F300	1 0 0 0 1	
4.098E-01	5.660E+01	100	D041	1 0 0 0 0	

731. $C_6H_6N_2O_2$
p-Nitroaniline
4-Amino-nitrobenzene
Benzenamine
4-Nitroaniline
p-Aminonitrobenzene
4-Nitrobenzenamine
RN: 100-01-6 **MP** (°C)**:** 146
MW: 138.13 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.754E-03	7.948E-01	20	B179	0 0 0 0 0	
2.823E-03	3.900E-01	20	H300	1 2 2 2 1	*sic*
2.815E-03	3.888E-01	20	T301	1 2 2 2 2	
3.020E-03	4.171E-01	25	B335	1 2 0 0 1	
4.344E-03	6.000E-01	25	F300	1 0 0 0 2	*sic*
5.370E-03	7.418E-01	25	L016	1 0 0 0 2	unit assumed
4.110E-03	5.677E-01	25.0	C026	0 0 0 0 0	
5.267E-03	7.275E-01	30	G029	1 0 2 2 2	
8.367E-03	1.156E+00	40.1	C026	0 0 0 0 0	

732. $C_6H_6N_2O_2$
2-Nitroaniline
o-Nitroaniline
1-Amino-2-nitrobenzene
2-Nitro-aniline
RN: 88-74-4 **MP** (°C)**:** 71.5
MW: 138.13 **BP** (°C)**:** 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.467E-03	8.932E-01	20	T301	1 2 2 2 2	
8.764E-03	1.211E+00	25.0	C026	0 0 0 0 0	
1.750E-02	2.417E+00	40.1	C026	0 0 0 0 0	
6.134E-03	8.473E-01	50	T301	1 2 2 2 2	average of 4
6.799E-03	9.391E-01	80	T301	1 2 2 2 2	average of 4

733. $C_6H_6N_2O_3$
5,5-Ethylenebarbituric acid
Spirocyclopropane-1′,5-barbituric acid
5,7-Diazaspiro[2.5]octane-4,6,8-trione
Cyclopropane-spirobarbiturate
RN: 6947-77-9 **MP** (°C)**:**
MW: 154.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.004E+00	25	P350	0 0 0 0 0	intrinsic

734. $C_6H_6N_2O_4$
1-Methylorotic acid
4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-
RN: 705-36-2 **MP** (°C)**:**
MW: 170.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.042E+01	20	N019	0 0 0 0 0	

735. $C_6H_6N_2O_4S$
m-Nitrobenzenesulfonamide
3-Nitrobenzenesulfonamide
RN: 121-52-8 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	4.448E-01	15	K024	1 2 1 1 2	

736. $C_6H_6N_2O_4S$
4-Nitrobenzenesulfonamide
p-Nitrobenzenesulfonamide
RN: 6325-93-5 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.066E-01	15	K024	1 2 1 1 2	

737. $C_6H_6N_2O_4S$
2-Nitrobenzenesulfonamide
o-Nitrobenzenesulfonamide
RN: 5455-59-4 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	3.235E-01	15	K024	1 2 1 1 2	

738. $C_6H_6N_4$
8-Methylpurine
1H-Purine, 8-methyl-
RN: 934-33-8 **MP** (°C)**:**
MW: 134.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.924E-01	5.263E+01	20	A022	1 0 0 0 0	

739. $C_6H_6N_4O$
8-Hydroxymethylpurine
Purine-8-methanol
RN: 6642-26-8 **MP** (°C)**:**
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.014E-02	4.525E+00	20	A022	1 2 0 0 0	
4.440E-01	6.667E+01	100	A082	1 2 0 0 0	

740. $C_6H_6N_4O_3$
9-Methyluric acid
1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-9-methyl-
*N*9-Methyluric acid
RN: 55441-71-9 **MP** (°C)**:**
MW: 182.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-03	5.461E-01	ns	B115	0 0 1 1 0	

741. $C_6H_6N_4O_3$
1-Methyluric acid
α-Methyluric acid
RN: 708-79-2 **MP** (°C)**:** 400
MW: 182.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	2.101E+00	ns	B115	0 0 1 1 0	ζ form
8.701E-03	1.585E+00	ns	B115	0 0 1 1 0	γ form
2.731E-02	4.975E+00	ns	B115	0 0 1 1 0	
2.754E-02	5.017E+00	ns	R427	0 0 0 0 0	

742. $C_6H_6N_4O_3S$
Niridazole
Nirodazole
RN: 61-57-4 **MP** (°C)**:** 261
MW: 214.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.068E-04	1.300E-01	25	A081	1 0 1 1 0	EFG
1.634E-04	3.500E-02	25	G051	1 0 1 1 0	pH 2

743. $C_6H_6N_4O_4$
5-Nitro-2-furaldehyde semicarbazone
Nitrofurazone
RN: 59-87-0 **MP** (°C)**:** 236
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.225E-04	1.630E-01	ns	B404	0 2 1 1 0	
1.201E-03	2.380E-01	ns	I310	0 0 0 0 0	
8.128E-04	1.611E-01	ns	R427	0 0 0 0 0	

744. $C_6H_6N_6$
2,4-Diaminopteridine
2:4-Diaminopteridine
RN: 1127-93-1 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.055E-03	3.332E-01	20	A019	2 2 1 1 2	
4.708E-02	7.634E+00	100	A019	1 2 1 1 1	

745. $C_6H_6N_6$
4,6-Diaminopteridine
4:6-Diaminopteridine
RN: 19167-60-3 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.569E-04	4.166E-02	20	A020	1 2 0 1 1	
6.554E-03	1.063E+00	100	A020	1 2 0 0 0	

746. $C_6H_6N_6$
4,7-Diaminopteridine
4:7-Diaminopteridine
RN: 771-41-5 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
1.233E-03	2.000E-01	20	A020	1 2 0 0 1	
2.049E-02	3.322E+00	100	A020	1 2 0 0 0	

747. $C_6H_6N_6$
4-Hydrazinopteridine
4(1H)-Pteridinone, hydrazone
RN: 77632-11-2 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
1.367E-02	2.217E+00	20	A083	1 2 0 0 0	
8.686E-02	1.408E+01	100	A083	1 2 0 0 0	

748. C_6H_6O
Phenol
Carbolic acid
Hydroxybenzene
RN: 108-95-2 **MP** (°C)**:** 40.85
MW: 94.11 **BP** (°C)**:** 182

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
7.164E-01	6.743E+01	0	A056	1 0 1 1 2	
7.136E-01	6.716E+01	0	B031	1 2 2 2 1	
7.164E-01	6.743E+01	0	L059	1 0 1 1 2	
6.858E-01	6.455E+01	8.60	C058	2 0 2 1 1	
7.321E-01	6.890E+01	10	A056	1 0 1 1 2	
7.321E-01	6.890E+01	10	L059	1 0 1 1 2	
8.080E-01	7.604E+01	15.1	A400	2 1 2 2 2	

(*continued*)

748. C_6H_6O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-01	6.279E+01	16	D041	1 0 0 0 1	
7.779E-01	7.322E+01	20	B031	1 2 2 2 1	
8.710E-01	8.197E+01	20	B179	0 0 0 0 0	
4.866E+00	4.580E+02	20	C052	1 2 1 1 2	*sic*
8.235E-01	7.750E+01	20	F300	1 0 0 0 2	
8.198E-01	7.715E+01	20	H003	1 2 2 1 2	
1.600E+00	1.506E+02	20	H306	1 0 1 2 1	
8.500E-01	8.000E+01	20	K119	1 0 0 0 2	
7.130E-01	6.710E+01	20	K301	2 2 1 1 2	
6.175E-01	5.811E+01	20	R087	0 0 0 0 0	0.15M NaCl
9.490E-01	8.931E+01	22.70	M135	1 2 1 1 2	
1.000E+00	9.411E+01	25	A021	1 2 1 1 0	
8.930E-01	8.405E+01	25	A400	2 1 2 2 2	
9.882E-01	9.300E+01	25	B060	2 0 1 1 1	
9.400E-01	8.847E+01	25	B316	0 0 0 0 0	
9.000E-01	8.470E+01	25	F044	1 0 0 0 1	
8.468E-01	7.970E+01	25	H003	1 2 2 1 2	
8.245E-01	7.759E+01	25	H028	2 0 2 0 2	
1.527E-01	1.437E+01	25	K129	2 1 2 2 2	
8.854E-01	8.333E+01	25	L022	1 0 0 0 0	
9.000E-01	8.470E+01	25	L088	1 0 0 0 1	
7.413E-01	6.977E+01	25	M041	1 1 0 0 1	
9.300E-01	8.753E+01	25	P031	0 0 0 0 0	
7.688E-01	7.236E+01	25	R041	0 0 0 0 0	
9.900E-01	9.317E+01	26.90	M135	1 2 1 1 2	
8.970E-01	8.442E+01	30	H003	1 2 2 1 2	
8.297E-01	7.809E+01	30	V009	1 0 0 0 1	
1.048E+00	9.863E+01	32.20	M135	1 2 1 1 2	
9.598E-01	9.033E+01	34	B063	1 2 2 1 2	
9.892E-01	9.310E+01	35	A400	2 1 2 2 2	
9.580E-01	9.016E+01	35	H003	1 2 2 1 2	
1.107E+00	1.042E+02	36.00	M135	1 2 1 1 2	
9.130E-01	8.592E+01	40	B031	1 2 2 2 1	
1.158E+00	1.090E+02	43.70	M135	1 2 1 1 2	
1.369E+00	1.288E+02	47.70	M135	1 2 1 1 2	
1.172E+00	1.103E+02	48.00	C058	2 0 2 1 2	
1.138E+00	1.071E+02	50	M041	1 1 0 0 2	
1.476E+00	1.389E+02	50.50	M135	1 2 1 1 2	
1.183E+00	1.113E+02	51.90	B063	1 2 2 1 2	
1.592E+00	1.498E+02	53.50	M135	1 2 1 1 2	
1.725E+00	1.623E+02	55.80	M135	1 2 1 1 2	
1.388E+00	1.306E+02	55.90	B063	1 2 2 1 2	
1.375E+00	1.295E+02	57.30	H003	1 2 2 1 2	
1.856E+00	1.747E+02	57.80	M135	1 2 1 1 2	
1.590E+00	1.497E+02	60	B031	1 2 2 2 2	
2.163E+00	2.036E+02	60.90	M135	1 2 1 1 2	
1.612E+00	1.518E+02	61.70	B063	1 2 2 1 2	
1.723E+00	1.621E+02	62.74	H003	1 2 2 1 2	
1.771E+00	1.667E+02	63.20	B063	1 2 2 1 2	

(*continued*)

748. C_6H_6O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+00	1.985E+02	65.40	B063	1 2 2 1 2	
3.064E+00	2.884E+02	65.50	B063	1 2 2 1 2	
2.567E+00	2.416E+02	65.55	B063	1 2 2 1 2	
2.767E+00	2.604E+02	65.60	B063	1 2 2 1 2	
2.388E+00	2.247E+02	65.79	H003	1 2 2 1 2	average of 2
2.590E+00	2.437E+02	65.84	H003	1 2 2 1 2	
2.624E+00	2.469E+02	65.86	H003	1 2 2 1 2	
2.536E+00	2.387E+02	65.90	H003	1 2 2 1 2	
2.818E+00	2.652E+02	66.0	H068	2 0 0 0 2	
2.397E+00	2.256E+02	66.01	H003	1 2 2 1 2	
1.734E+00	1.632E+02	66.30	C058	2 0 2 1 2	
8.243E-01	7.758E+01	ns	A406	0 0 0 0 1	
8.594E-01	8.088E+01	ns	N330	2 2 2 1 2	
8.710E-01	8.197E+01	ns	R427	0 0 0 0 0	
8.043E-01	7.570E+01	rt	N051	0 0 2 1 2	average of 3

749. $C_6H_6O_2$

Hydroquinone
Hydrochinon
Hydroquinol

RN: 123-31-9 **MP** (°C)**:** 173.5
MW: 110.11 **BP** (°C)**:** 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.493E-01	3.846E+01	0	M043	1 0 0 0 1	
4.653E-01	5.123E+01	10	M043	1 0 0 0 1	
4.904E-01	5.400E+01	15	F300	1 0 0 0 1	
5.077E-01	5.590E+01	17.70	L065	1 0 0 0 2	0.01N HCl
5.087E-01	5.601E+01	17.90	L065	1 0 0 0 2	0.01N HCl
5.101E-01	5.617E+01	17.95	L065	1 0 0 0 2	0.01N HCl
5.103E-01	5.619E+01	18	L064	2 2 2 1 2	0.01N HCl
6.100E-01	6.716E+01	20	M043	1 0 0 0 1	
6.357E-01	7.000E+01	22.5	G301	0 0 0 0 0	
6.180E-01	6.805E+01	23.75	L064	2 2 2 1 2	0.01N HCl
6.450E-01	7.102E+01	25	G033	1 0 1 1 2	
7.283E-01	8.020E+01	25	K033	1 0 0 1 2	
6.660E-01	7.334E+01	25	K040	1 0 2 1 2	
7.955E-01	8.759E+01	30	M043	1 0 0 0 1	
1.045E+00	1.150E+02	40	M043	1 0 0 0 1	
2.354E+00	2.593E+02	60	M043	1 0 0 0 1	
5.694E+00	6.270E+02	75.3	W038	2 2 2 1 2	
4.251E+00	4.681E+02	80	M043	1 0 0 0 1	
7.528E+00	8.289E+02	81.9	W038	2 2 2 1 2	
6.034E+00	6.644E+02	100	M043	1 0 0 0 2	
1.961E+01	2.159E+03	114.6	W038	2 2 2 1 2	
2.180E+01	2.400E+03	120.3	W038	2 2 2 1 2	
2.728E+01	3.004E+03	131.7	W038	2 2 2 1 2	

(*continued*)

749. $C_6H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.942E+01	3.239E+03	136.0	W038	2 2 2 1 2	
3.353E+01	3.692E+03	141.8	W038	2 2 2 1 2	
3.621E+01	3.987E+03	147.2	W038	2 2 2 1 2	
6.026E-01	6.635E+01	ns	R427	0 0 0 0 0	
6.084E-01	6.699E+01	rt	D021	0 0 1 1 2	

750. $C_6H_6O_2$

Pyrocatechol
Brenzkatechin
Catechol

RN: 120-80-9 **MP** (°C)**:** 105
MW: 110.11 **BP** (°C)**:** 245.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.824E+00	3.110E+02	20	F300	1 0 0 0 2	
2.823E+00	3.108E+02	20	M043	1 0 0 0 2	
4.190E+00	4.614E+02	25	K040	1 0 2 1 2	
5.743E+00	6.324E+02	40	M043	1 0 0 0 2	
1.278E+01	1.408E+03	41.2	W038	2 2 2 1 2	
2.061E+01	2.270E+03	56.7	W038	2 2 2 1 2	
2.068E+01	2.278E+03	57.1	W038	2 2 2 1 2	
7.308E+00	8.047E+02	60	M043	1 0 0 0 2	
2.617E+01	2.882E+03	66.2	W038	2 2 2 1 2	
8.337E+00	9.180E+02	80	M043	1 0 0 0 2	
8.974E+00	9.882E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	104.5	W038	2 2 2 1 2	
2.823E+00	3.108E+02	rt	D021	0 0 1 1 2	

751. $C_6H_6O_2$

Resorcinol
Resorcin

RN: 108-46-3 **MP** (°C)**:** 110.0
MW: 110.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E+00	3.748E+02	0	M022	1 0 0 0 2	
3.617E+00	3.983E+02	0	M043	1 0 0 0 2	
2.784E+00	3.066E+02	3.70	L090	1 0 0 1 2	
4.173E+00	4.595E+02	10	M043	1 0 0 0 1	
5.413E+00	5.960E+02	12.50	F300	1 0 0 0 2	
3.186E+00	3.508E+02	14.20	L090	1 0 0 1 2	
3.359E+00	3.699E+02	19.50	L090	1 0 0 1 2	
4.576E+00	5.038E+02	20	M022	1 0 0 0 2	
5.009E+00	5.516E+02	20	M043	1 0 0 0 2	
6.515E+00	7.174E+02	25	K040	1 0 2 1 2	

(*continued*)

751. $C_6H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.330E+00	6.970E+02	30	F300	1 0 0 0 2	
5.718E+00	6.296E+02	30	M043	1 0 0 0 2	
3.679E+00	4.051E+02	32.50	L090	1 0 0 1 2	
1.464E+01	1.612E+03	33.61	W038	2 2 2 1 2	
5.641E+00	6.211E+02	40	M022	1 0 0 0 2	
6.287E+00	6.923E+02	40	M043	1 0 0 0 2	
1.843E+01	2.030E+03	44.5	W038	2 2 2 1 2	
2.042E+01	2.249E+03	49.3	W038	2 2 2 1 2	
2.100E+01	2.312E+03	50.4	W038	2 2 2 1 2	
6.465E+00	7.119E+02	60	M022	1 0 0 0 2	
7.228E+00	7.959E+02	60	M043	1 0 0 0 2	
2.701E+01	2.974E+03	64.4	W038	2 2 2 1 2	
2.997E+01	3.300E+03	70.7	W038	2 2 2 1 2	
7.106E+00	7.825E+02	80	M022	1 0 0 0 2	
7.844E+00	8.638E+02	80	M043	1 0 0 0 2	
3.516E+01	3.871E+03	80.5	W038	2 2 2 1 2	
4.008E+01	4.414E+03	88.5	W038	2 2 2 1 2	
7.592E+00	8.360E+02	100	M022	1 0 0 0 2	
8.299E+00	9.138E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	109.4	W038	2 2 2 1 2	
4.608E+00	5.074E+02	rt	D021	0 0 1 1 2	

752. $C_6H_6O_3$

Maltol
3-Hydroxy-2-methyl-4-pyrone
Hydroxymethylpyrone
Palatone

RN: 118-71-8 **MP** (°C)**:** 161.5
MW: 126.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.643E-02	1.090E+01	15	F300	1 0 0 0 2	

753. $C_6H_6O_3$

Methyl furoate
5-Methyl-brenzschleimsaeure
5-Methylfuroic acid

RN: 611-13-2 **MP** (°C)**:**
MW: 126.11 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	1.860E+01	20	F300	1 0 0 0 2	

754. $C_6H_6O_3$

Phloroglucinol
1,3,5-Benzenetriol
1,3,5-Trihydroxybenzene
1,3,5-THB

RN: 108-73-6 **MP** (°C)**:** 218.0
MW: 126.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.405E-02	1.060E+01	20	F300	1 0 0 0 2	
8.860E-02	1.117E+01	rt	D021	0 0 1 1 2	

755. $C_6H_6O_3$

Pyrogallol
1,2,3-Trihydroxybenzene
1,2,3-Benzenetriol
Brown AP
Fourrine 85

RN: 87-66-1 **MP** (°C)**:** 131
MW: 126.11 **BP** (°C)**:** 309

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	3.000E+02	13	F300	1 0 0 0 0	average
3.013E+00	3.800E+02	25	F300	1 0 0 0 1	
4.020E+00	5.070E+02	25	K040	1 0 2 1 2	

756. $C_6H_6O_3S$

Benzenesulfonic acid
Benzolsulfosaeure

RN: 98-11-3 **MP** (°C)**:** 43
MW: 158.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.088E+00	4.885E+02	31.4	T023	1 2 2 1 2	
3.109E+00	4.917E+02	42.6	T023	1 2 2 1 2	
3.136E+00	4.960E+02	56.0	T023	1 2 2 1 2	
3.154E+00	4.989E+02	61.3	T023	1 2 2 1 2	

757. $C_6H_6O_3S.H_2O$

Benzenesulfonic acid (monohydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 176.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E+00	4.478E+02	21.3	T023	1 2 2 1 2	
2.568E+00	4.525E+02	31.0	T023	1 2 2 1 2	
2.770E+00	4.881E+02	32.6	T023	1 2 2 1 2	

(*continued*)

757. $C_6H_6O_3S.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.598E+00	4.577E+02	39.5	T023	1 2 2 1 2	
2.751E+00	4.846E+02	39.8	T023	1 2 2 1 2	
2.722E+00	4.796E+02	49.0	T023	1 2 2 1 2	
2.641E+00	4.654E+02	49.0	T023	1 2 2 1 2	
2.682E+00	4.726E+02	52.4	T023	1 2 2 1 2	

758. $C_6H_6O_3S.2.5H_2O$

Benzenesulfonic acid (2.5 hydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 203.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.281E+02	–4.0	T023	1 2 2 1 2	
2.122E+00	4.312E+02	–3.3	T023	1 2 2 1 2	
2.150E+00	4.370E+02	–2.3	T023	1 2 2 1 2	
2.131E+00	4.331E+02	–2.5	T023	1 2 2 1 2	

759. $C_6H_6O_3S.2H_2O$

Benzenesulfonic acid (dihydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E+00	4.370E+02	2.2	T023	1 2 2 1 2	
2.265E+00	4.399E+02	7.5	T023	1 2 2 1 2	
2.289E+00	4.446E+02	13.7	T023	1 2 2 1 2	
2.297E+00	4.460E+02	15.1	T023	1 2 2 1 2	

760. $C_6H_6O_3S.3H_2O$

Benzenesulfonic acid (trihydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 212.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E+00	3.586E+02	–40.8	T023	1 2 2 1 2	
1.766E+00	3.748E+02	–29.0	T023	1 2 2 1 2	
1.842E+00	3.909E+02	–18.5	T023	1 2 2 1 2	
1.922E+00	4.078E+02	–10.0	T023	1 2 2 1 2	
1.975E+00	4.191E+02	–5.9	T023	1 2 2 1 2	
2.011E+00	4.267E+02	–4.7	T023	1 2 2 1 2	

761. $C_6H_6O_4$
Muconic acid
Muconsaeure
RN: 505-70-4 **MP** (°C)**:**
MW: 142.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.407E-03	2.000E-01	20	F300	1 0 0 0 2	

762. $C_6H_7F_3N_4OS$
Thiazafluron
Urea, *N*,*N*′-dimethyl-*N*-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-
RN: 25366-23-8 **MP** (°C)**:** 136.5
MW: 240.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.724E-03	2.096E+00	20	E048	1 2 1 1 2	
8.742E-03	2.100E+00	20	M161	1 0 0 0 1	

763. C_6H_7N
Aniline
Aminobenzene
C.I. Oxidation base 1
Aminophen
Kyanol
RN: 62-53-3 **MP** (°C)**:** –6.3
MW: 93.13 **BP** (°C)**:** 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.531E-01	3.288E+01	8.60	C058	2 0 2 1 1	
3.877E-01	3.611E+01	13.8	K119	1 0 0 0 2	
3.747E-01	3.490E+01	18	F300	1 0 0 0 2	
3.818E-01	3.556E+01	18.15	P057	0 0 0 0 0	
3.612E-01	3.364E+01	22	H072	1 0 1 1 2	
3.930E-01	3.660E+01	22.5	G301	0 0 0 0 0	
3.931E-01	3.661E+01	25	B019	1 0 1 2 0	
3.931E-01	3.661E+01	25	B092	2 1 1 1 2	
4.000E-01	3.725E+01	25	F044	1 0 0 0 1	
3.791E-01	3.531E+01	25	G323	2 2 2 2 2	
3.800E-01	3.539E+01	25	H028	2 0 2 0 2	
3.791E-01	3.531E+01	25	H078	1 2 1 0 2	
3.650E-01	3.399E+01	25	M116	2 1 1 1 2	
3.731E-01	3.475E+01	25.40	C058	2 0 2 1 1	
3.930E-01	3.660E+01	26.70	L095	2 2 1 1 2	
4.229E-01	3.939E+01	48.00	C058	2 0 2 1 1	
4.328E-01	4.031E+01	50	G323	2 2 2 2 2	
5.016E-01	4.671E+01	60	B092	2 1 1 1 2	
5.016E-01	4.671E+01	66.30	C058	2 0 2 1 1	
7.025E-01	6.542E+01	96.70	C058	2 0 2 1 1	
3.801E-01	3.540E+01	ns	A406	0 0 0 0 1	

764. C_6H_7NO

m-Aminophenol
3-Aminophenol

RN: 591-27-5 **MP** (°C)**:** 125
MW: 109.13 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.797E-01	1.961E+01	10	M043	1 0 0 0 1	
2.291E-01	2.500E+01	20	F300	1 0 0 0 1	
2.409E-01	2.629E+01	20	M043	1 0 0 0 1	
3.355E-01	3.661E+01	30	M043	1 0 0 0 1	
3.261E-01	3.559E+01	32.6	S120	1 2 1 1 2	
4.859E-01	5.303E+01	40	M043	1 0 0 0 1	
6.788E-01	7.407E+01	47.9	S120	1 2 1 1 2	
8.850E-01	9.658E+01	53.0	S120	1 2 1 1 2	
1.590E+00	1.736E+02	60	M043	1 0 0 0 1	
1.406E+00	1.535E+02	60.4	S120	1 2 1 1 2	
2.148E+00	2.344E+02	66.4	S120	1 2 1 1 2	
2.627E+00	2.866E+02	68.9	S120	1 2 1 1 2	
2.927E+00	3.194E+02	70.2	S120	1 2 1 1 2	
3.161E+00	3.450E+02	71.5	S120	1 2 1 1 2	
3.410E+00	3.721E+02	73.2	S120	1 2 1 1 2	
3.737E+00	4.078E+02	77.2	S120	1 2 1 1 2	
6.752E+00	7.368E+02	80	M043	1 0 0 0 2	
4.098E+00	4.472E+02	85.2	S120	1 2 1 1 2	
4.311E+00	4.705E+02	96.0	S120	1 2 1 1 2	
8.291E+00	9.048E+02	100	M043	1 0 0 0 2	

765. C_6H_7NO

o-Aminophenol
2-Amino-phenol

RN: 95-55-6 **MP** (°C)**:** 172
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-01	1.700E+01	0	F300	1 0 0 0 1	
1.532E-01	1.672E+01	0	M043	1 0 0 0 1	
1.709E-01	1.865E+01	10	M043	1 0 0 0 1	
1.797E-01	1.961E+01	20	M043	1 0 0 0 1	
1.973E-01	2.153E+01	30	M043	1 0 0 0 1	
2.148E-01	2.344E+01	40	M043	1 0 0 0 1	
2.409E-01	2.629E+01	60	M043	1 0 0 0 1	
2.669E-01	2.913E+01	80	M043	1 0 0 0 1	
2.686E-01	2.931E+01	80.8	S120	1 2 1 1 1	
3.558E-01	3.883E+01	88.0	S120	1 2 1 1 1	
5.995E-01	6.542E+01	100	M043	1 0 0 0 1	

766. C_6H_7NO
p-Aminophenol
4-Aminophenol
RN: 123-30-8 **MP** (°C)**:** 190
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-01	1.100E+01	0	F300	1 0 0 0 1	
9.970E-02	1.088E+01	0	M043	1 0 0 0 1	
1.176E-01	1.283E+01	10	M043	1 0 0 0 1	
1.443E-01	1.575E+01	20	M043	1 0 0 0 1	
1.709E-01	1.865E+01	30	M043	1 0 0 0 1	
2.060E-01	2.248E+01	40	M043	1 0 0 0 1	
2.678E-01	2.922E+01	59.0	S120	1 2 1 1 1	
3.184E-01	3.475E+01	60	M043	1 0 0 0 1	
5.544E-01	6.050E+01	77.0	S120	1 2 1 1 1	
6.709E-01	7.322E+01	80	M043	1 0 0 0 1	
8.399E-01	9.165E+01	86.7	S120	1 2 1 1 1	
1.497E+00	1.634E+02	96.6	S120	1 2 1 1 1	
2.475E+00	2.701E+02	100	M043	1 0 0 0 1	

767. C_6H_7NO
Phenylhydroxylamine
Phenylhydroxylamin
RN: 100-65-2 **MP** (°C)**:** 82
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-01	2.000E+01	5	F300	1 0 0 0 0	
8.247E-01	9.000E+01	100	F300	1 0 0 0 0	

768. $C_6H_7NO_2S$
Benzenesulfonamide
Benzolsulfosaeure-amid
RN: 98-10-2 **MP** (°C)**:** 151
MW: 157.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	2.515E+00	15	K024	1 2 1 1 2	
2.736E-02	4.300E+00	16	F300	1 0 0 0 1	

769. $C_6H_7NO_3S$
Orthanilic acid
Orthanilsaeure
RN: 88-21-1 **MP** (°C)**:** 325
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.525E-02	1.130E+01	8.25	P038	1 1 2 1 2	monohydrate
7.535E-02	1.305E+01	12.3	P038	1 1 2 1 2	monohydrate
8.459E-02	1.465E+01	15.55	P038	1 1 2 1 2	anhydrate
8.776E-02	1.520E+01	16.75	P038	1 1 2 1 2	anhydrate
1.114E-01	1.930E+01	25	P038	1 1 2 1 2	anhydrate
1.738E-01	3.010E+01	41.3	P038	1 1 2 1 2	anhydrate
2.477E-01	4.290E+01	55.0	P038	1 1 2 1 2	anhydrate
3.672E-01	6.360E+01	70.0	P038	1 1 2 1 2	anhydrate
5.185E-01	8.980E+01	85.0	P038	1 1 2 1 2	anhydrate
4.585E-02	7.940E+00	.0	P038	1 1 2 1 2	monohydrate

770. $C_6H_7NO_3S$
Sulfanilic acid
4-Aminobenzenesulfonic acid
Sulfanilsaeure
RN: 121-57-3 **MP** (°C)**:** 122
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-02	6.359E+00	0	D077	1 0 0 1 1	
2.587E-02	4.480E+00	0	M043	1 0 0 0 1	
4.810E-02	8.330E+00	10	D077	1 0 0 1 1	
4.850E-02	8.400E+00	10	F300	1 0 0 0 1	
4.583E-02	7.937E+00	10	M043	1 0 0 0 1	
6.169E-02	1.068E+01	20	D077	1 0 0 1 2	
5.774E-02	1.000E+01	20	F300	1 0 0 0 1	
6.395E-02	1.108E+01	20	M043	1 0 0 0 2	
8.477E-02	1.468E+01	30	D077	1 0 0 1 2	
1.115E-01	1.932E+01	40	D077	1 0 0 1 2	
1.109E-01	1.920E+01	40	F300	1 0 0 0 2	
1.149E-01	1.990E+01	40	M043	1 0 0 0 2	
1.414E-01	2.449E+01	50	D077	1 0 0 1 2	
1.736E-01	3.007E+01	60	D077	1 0 0 1 2	
1.687E-01	2.922E+01	60	M043	1 0 0 0 2	
2.159E-01	3.740E+01	69.9	P038	1 0 2 1 2	anhydrate
2.103E-01	3.642E+01	70	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	M043	1 0 0 0 2	
2.737E-01	4.740E+01	85.0	P038	1 0 2 1 2	anhydrate
3.031E-01	5.249E+01	90	D077	1 0 0 1 2	
3.610E-01	6.253E+01	100	D077	1 0 0 1 2	
3.851E-01	6.670E+01	100	F300	1 0 0 0 2	
3.610E-01	6.253E+01	100	M043	1 0 0 0 2	
6.075E-02	1.052E+01	ns	K076	0 0 0 0 2	

771. $C_6H_7NO_3S$
Metanilic acid
3-Aminobenzenesulfonic acid
m-Sulfanilic acid
RN: 121-47-1 **MP** (°C)**:** >300
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.901E-02	1.022E+01	7.75	P038	1 2 2 1 2	anhydrate
7.622E-02	1.320E+01	16.75	P038	1 2 2 1 2	anhydrate
9.440E-02	1.635E+01	24.95	P038	1 2 2 1 2	anhydrate
1.383E-01	2.395E+01	40.0	P038	1 2 2 1 2	anhydrate
1.975E-01	3.420E+01	55.0	P038	1 2 2 1 2	anhydrate
2.714E-01	4.700E+01	70.0	P038	1 2 2 1 2	anhydrate
4.561E-02	7.900E+00	.0	P038	1 2 2 1 2	anhydrate

772. $C_6H_7NO_3S.1.5H_2O$
Metanilic acid (sesquihydrate)
3-Aminobenzenesulfonic acid (sesquihydrate)
RN: 121-47-1 **MP** (°C)**:**
MW: 200.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.041E-02	1.610E+01	8.35	P038	1 2 2 1 2	
1.119E-01	2.240E+01	15.55	P038	1 2 2 1 2	
1.184E-01	2.370E+01	16.8	P038	1 2 2 1 2	
3.247E-01	6.500E+01	85.0	P038	1 2 2 1 2	
5.344E-02	1.070E+01	.0	P038	1 2 2 1 2	

773. $C_6H_7NO_4S$
2-Aminophenol-4-sulfonic acid
2-Amino-phenol-sulfosaeure-(4)
RN: 98-37-3 **MP** (°C)**:** >300
MW: 189.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-02	1.000E+01	14	F300	1 0 0 0 0	

774. $C_6H_7NO_4S$
4-Aminophenol-2-sulfonic acid
4-Amino-phenol-sulfosaeure-(2)
RN: 2835-04-3 **MP** (°C)**:**
MW: 189.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	7.000E-01	14	F300	1 0 0 0 0	

775. $C_6H_7N_3O$
Isoniazid
Isonicotinic acid hydrazide
laniazid
RN: 54-85-3 **MP** (°C)**:** 171
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.813E-01	1.071E+02	20	I307	0 0 0 0 0	
8.955E-01	1.228E+02	25	B187	0 0 0 0 0	
1.458E+00	2.000E+02	37	I307	0 0 0 0 0	
1.505E+00	2.063E+02	40	B187	0 0 0 0 0	
9.115E-01	1.250E+02	ns	K444	0 0 0 0 0	

776. $C_6H_7N_3O_3$
Orotic acid methylamide
Orotamide, *N*-methyl-
RN: 1009-04-7 **MP** (°C)**:** 284–286
MW: 169.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.420E-01	5.785E+01	–4	N018	0 0 0 0 0	
6.840E-01	1.157E+02	16	N018	0 0 0 0 0	
8.340E-01	1.411E+02	25	N018	0 0 0 0 0	

777. $C_6H_7N_7$
2,4,7-Triaminopteridine
2:4:7-Triaminopteridine
RN: 14439-13-5 **MP** (°C)**:**
MW: 177.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.254E-03	2.222E-01	20	A020	1 2 0 0 1	
2.808E-02	4.975E+00	100	A020	1 2 0 0 0	

778. $C_6H_7N_7$
4,6,7-Triaminopteridine
4:6:7-Triaminopteridine
RN: 19167-62-5 **MP** (°C)**:**
MW: 177.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.515E-04	7.999E-02	20	A020	1 2 0 1 1	
1.252E-02	2.217E+00	100	A020	1 2 0 0 1	

779. $C_6H_7O_2P$
Phenylphosphinic acid
Phenyl-phosphinigsaeure
RN: 1779-48-2 **MP** (°C)**:** 84
MW: 142.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.757E-01	6.760E+01	14	F300	1 0 0 0 2	
9.460E+00	1.344E+03	24.63	W422	0 0 0 0 0	
1.109E+01	1.576E+03	27.09	W422	0 0 0 0 0	
1.294E+01	1.839E+03	29.24	W422	0 0 0 0 0	
1.593E+01	2.264E+03	32.06	W422	0 0 0 0 0	
2.177E+01	3.093E+03	36.77	W422	0 0 0 0 0	
3.047E+01	4.330E+03	39.68	W422	0 0 0 0 0	
4.843E+00	6.881E+02	100	F300	1 0 0 0 2	

780. $C_6H_7O_3P$
Phenylphosphonic acid
Phenylphosphonsaeure
RN: 1571-33-1 **MP** (°C)**:** 164.5
MW: 158.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.900E+02	15	F300	1 0 0 0 2	
1.202E+00	1.901E+02	ns	R427	0 0 0 0 0	

781. $C_6H_7O_3As$
Benzenearsonic acid
Phenylarsonsaeure
RN: 98-05-5 **MP** (°C)**:** 160
MW: 202.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.564E-01	3.160E+01	28	F300	1 0 0 0 2	
9.899E-01	2.000E+02	84	F300	1 0 0 0 1	

782. C_6H_8
1,4-Cyclohexadiene
1,4-Dihydrobenzene
RN: 628-41-1 **MP** (°C)**:** –49.2
MW: 80.13 **BP** (°C)**:** 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-02	8.512E-01	4.8	L007	2 2 1 2 2	
1.062E-02	8.512E-01	5.1	L007	2 1 1 1 2	
1.195E-02	9.576E-01	14.8	L007	2 2 1 2 2	

(*continued*)

782. C_6H_8 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-02	9.576E-01	15.2	L007	2 1 1 1 2	
8.002E-03	6.412E-01	20	M337	2 1 2 2 2	
1.167E-02	9.353E-01	24.8	L007	2 2 1 2 2	
8.736E-03	7.000E-01	25	M001	2 1 2 2 2	
1.167E-02	9.353E-01	25.1	L007	2 1 1 1 2	
1.201E-02	9.625E-01	34.8	L007	2 2 1 2 2	
1.201E-02	9.625E-01	35.2	L007	2 1 1 1 2	
1.259E-02	1.009E+00	44.8	L007	2 2 1 2 2	
1.259E-02	1.009E+00	45.2	L007	2 1 1 1 2	

783. $C_6H_8ClN_7O$
Amiloride
RN: 2609-46-3 **MP** (°C)**:**
MW: 229.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.531E-04	1.500E-01	22.5	B422	0 0 0 0 0	
2.870E+00	6.590E+02	25	B443	0 0 0 0 0	

784. $C_6H_8N_2$
2,5-Dimethylpyrazine
2,5-Dimethyl-pyrazin
RN: 123-32-0 **MP** (°C)**:** 63
MW: 108.14 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		25	D425	0 0 0 0 0	

785. $C_6H_8N_2$
m-Phenylenediamine
m-Phenylendiamin
RN: 108-45-2 **MP** (°C)**:** 63
MW: 108.14 **BP** (°C)**:** 283

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.409E-01	8.012E+01	.3	S115	1 2 1 1 2	α form
2.928E-01	3.166E+01	.3	S115	1 2 1 1 2	β form
1.038E+00	1.122E+02	4.6	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	9.3	S115	1 2 1 1 2	α form
1.618E+00	1.750E+02	11.7	S115	1 2 1 1 2	α form
7.806E-01	8.442E+01	14.3	S115	1 2 1 1 2	β form
2.285E+00	2.472E+02	16.1	S115	1 2 1 1 2	α form
2.671E+00	2.889E+02	17.3	S115	1 2 1 1 2	α form
1.038E+00	1.122E+02	18.3	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	18.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	19.9	S115	1 2 1 1 2	α form

(*continued*)

785. $C_6H_8N_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.537E+00	3.825E+02	20.8	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	22.0	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	22.7	S115	1 2 1 1 2	α form
1.480E+00	1.600E+02	23.1	S115	1 2 1 1 2	β form
1.618E+00	1.750E+02	24.1	S115	1 2 1 1 2	β form
1.918E+00	2.074E+02	25.1	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	26.0	S115	1 2 1 1 2	α form
2.285E+00	2.472E+02	26.3	S115	1 2 1 1 2	β form
2.671E+00	2.889E+02	27.1	S115	1 2 1 1 2	β form
2.815E+00	3.044E+02	27.1	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	27.9	S115	1 2 1 1 2	β form
4.085E+00	4.418E+02	28.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	29.0	S115	1 2 1 1 2	β form
3.537E+00	3.825E+02	29.1	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	30.2	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	31.5	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	32.6	S115	1 2 1 1 2	α form
4.085E+00	4.418E+02	32.8	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	34.4	S115	1 2 1 1 2	β form
4.439E+00	4.800E+02	43.5	S115	1 2 1 1 2	α form
4.549E+00	4.919E+02	53.6	S115	1 2 1 1 2	α form
4.586E+00	4.960E+02	57.6	S115	1 2 1 1 2	α form
4.623E+00	5.000E+02	62.8	S115	1 2 1 1 2	α form

786. $C_6H_8N_2$

o-Phenylenediamine
o-Phenylendiamin

RN: 95-54-5 **MP** (°C)**:** 102–103
MW: 108.14 **BP** (°C)**:** 257

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.876E-01	3.110E+01	20	T301	1 2 2 2 2	
3.763E-01	4.070E+01	35	F300	1 0 0 0 2	
3.599E-01	3.892E+01	35.1	S115	1 2 1 1 2	
5.110E-01	5.527E+01	45.8	S115	1 2 1 1 2	
9.804E-01	1.060E+02	56.3	S115	1 2 1 1 2	
1.458E+00	1.577E+02	61.3	S115	1 2 1 1 2	
1.755E+00	1.898E+02	62.8	S115	1 2 1 1 2	
2.218E+00	2.398E+02	64.2	S115	1 2 1 1 2	
2.948E+00	3.188E+02	66.1	S115	1 2 1 1 2	
3.558E+00	3.847E+02	67.7	S115	1 2 1 1 2	
3.955E+00	4.277E+02	71.3	S115	1 2 1 1 2	
4.338E+00	4.691E+02	80.8	S115	1 2 1 1 2	
4.476E+00	4.841E+02	88.1	S115	1 2 1 1 2	
4.533E+00	4.902E+02	91.7	S115	1 2 1 1 2	
4.570E+00	4.942E+02	95.5	S115	1 2 1 1 2	

787. $C_6H_8N_2$
p-Phenylenediamine
1,4-Phenylenediamine
RN: 106-50-3 **MP** (°C)**:** 141
MW: 108.14 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.880E-02	1.068E+01	3.6	S115	1 2 1 1 2	
3.299E-01	3.568E+01	23.7	S115	1 2 1 1 2	
4.180E-01	4.520E+01	25	F300	1 0 0 0 2	
8.292E-01	8.967E+01	37.8	S115	1 2 1 1 2	
1.460E+00	1.579E+02	49.9	S115	1 2 1 1 2	
1.978E+00	2.140E+02	59.2	S115	1 2 1 1 2	
2.368E+00	2.561E+02	64.6	S115	1 2 1 1 2	
2.724E+00	2.945E+02	69.2	S115	1 2 1 1 2	
3.155E+00	3.412E+02	75.5	S115	1 2 1 1 2	
3.432E+00	3.711E+02	80.3	S115	1 2 1 1 2	
3.809E+00	4.119E+02	88.5	S115	1 2 1 1 2	
4.055E+00	4.385E+02	95.9	S115	1 2 1 1 2	
1.500E-05	1.622E-03	98.59	M180	0 0 2 2 0	EFG
2.500E-05	2.704E-03	111.46	M180	0 0 2 2 0	EFG
4.000E-05	4.326E-03	117.47	M180	0 0 2 2 0	EFG
4.500E-05	4.866E-03	122.10	M180	0 0 2 2 0	EFG
5.000E-05	5.407E-03	126.84	M180	0 0 2 2 0	EFG
7.000E-05	7.570E-03	133.34	M180	0 0 2 2 0	EFG

788. $C_6H_8N_2OS$
5,6-Dimethyl-2-thiouracil
4(1H)-Pyrimidinone, 2,3-dihydro-5,6-dimethyl-2-thioxo-
5,6-Dimethylthiouracil
RN: 28456-54-4 **MP** (°C)**:**
MW: 156.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.790E-03	1.373E+00	25	G016	1 2 1 2 2	intrinsic

789. $C_6H_8N_2O_2$
N,N-1,3-Dimethyluracil
1,3-Dimethyl-2,4-pyrimidinedione
*N*1,*N*3-Dimethyluracil
N,N′-Dimethyluracil
1,3-Dimethyluracil
RN: 874-14-6 **MP** (°C)**:**
MW: 140.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.568E+00	5.000E+02	ns	B177	0 0 0 0 2	

790. $C_6H_8N_2O_2S$
o-Aminobenzenesulfonamide
Orthanilamide
RN: 3306-62-5 **MP** (°C)**:**
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-02	6.458E+00	23	K034	2 2 2 2 1	
3.865E-02	6.655E+00	24	K034	2 2 2 2 1	
4.323E-02	7.444E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	28	K034	2 2 2 2 1	
5.237E-02	9.018E+00	30.5	K034	2 2 2 2 1	
5.806E-02	9.999E+00	33	K034	2 2 2 2 2	
6.034E-02	1.039E+01	34	K034	2 2 2 2 2	
6.375E-02	1.098E+01	35.5	K034	2 2 2 2 2	
6.886E-02	1.186E+01	37	K034	2 2 2 2 2	
6.829E-02	1.176E+01	37	K034	2 2 2 2 2	
8.356E-02	1.439E+01	42	K034	2 2 2 2 2	
9.707E-02	1.672E+01	46	K034	2 2 2 2 2	
1.139E-01	1.961E+01	50	K034	2 2 2 2 2	

791. $C_6H_8N_2O_2S$
m-Aminobenzenesulfonamide
Metanilamide
m-Amidobenzenesulfonamide
RN: 98-18-0 **MP** (°C)**:**
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.545E-02	1.127E+01	23	K034	2 2 2 2 2	
6.942E-02	1.196E+01	24	K034	2 2 2 2 2	
7.678E-02	1.322E+01	26	K034	2 2 2 2 2	
8.469E-02	1.458E+01	28	K034	2 2 2 2 2	
1.077E-01	1.855E+01	33	K034	2 2 2 2 2	
1.244E-01	2.143E+01	35.5	K034	2 2 2 2 2	
1.339E-01	2.306E+01	37	K034	2 2 2 2 2	
1.461E-01	2.515E+01	39	K034	2 2 2 2 2	
1.697E-01	2.922E+01	42	K034	2 2 2 2 2	
2.072E-01	3.568E+01	46	K034	2 2 2 2 2	
2.543E-01	4.379E+01	50	K034	2 2 2 2 2	

792. $C_6H_8N_2O_2S$

Benzenesulfamide
Sulfanilamide
Sulfanilsaeure-amid
p-Aminobenzenesulphonamide

RN: 63-74-1 **MP** (°C)**:** 165
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	1	A047	1 0 0 0 0	EFG
1.057E-02	1.820E+00	4.40	B147	1 2 1 1 2	
1.458E-02	2.510E+00	10.20	B147	1 2 1 1 2	
1.957E-02	3.370E+00	15	B147	1 2 1 1 2	
2.323E-02	4.000E+00	15	F300	1 0 0 0 0	
2.660E-02	4.581E+00	15	K024	1 2 1 1 2	
2.241E-02	3.860E+00	15	S147	1 2 2 2 2	hydrate
2.889E-02	4.975E+00	16	A047	1 0 0 0 0	EFG
2.439E-02	4.200E+00	16	H114	1 0 0 0 2	
2.700E-02	4.650E+00	20	B147	1 2 1 1 2	
3.463E-02	5.964E+00	20	D041	1 0 0 0 0	
4.149E-02	7.145E+00	20	F073	1 2 2 2 2	
2.903E-02	5.000E+00	20	F300	1 0 0 0 0	
3.020E-02	5.200E+00	20	S147	1 2 2 2 2	hydrate
3.693E-02	6.359E+00	23	K034	2 2 2 2 1	
3.979E-02	6.853E+00	24	K034	2 2 2 2 1	
3.484E-02	6.000E+00	25	B147	1 2 1 1 2	
4.855E-02	8.360E+00	25	C102	2 0 2 2 2	
4.550E-02	7.835E+00	25	M116	2 1 1 1 2	
4.274E-02	7.360E+00	25	M440	0 0 0 0 0	
4.820E-02	8.300E+00	25	P015	0 0 0 0 0	
4.216E-02	7.260E+00	25	S147	1 2 2 2 2	hydrate
4.437E-02	7.641E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	27	K034	2 2 2 2 1	
5.008E-02	8.625E+00	28	K034	2 2 2 2 1	
4.762E-02	8.200E+00	30	B147	1 2 1 1 2	
5.633E-02	9.700E+00	30	S147	1 2 2 2 2	hydrate
5.806E-02	9.999E+00	30.5	K034	2 2 2 2 2	
6.318E-02	1.088E+01	31	A047	1 0 0 0 0	EFG
6.205E-02	1.068E+01	31.7	K034	2 2 2 2 2	
6.829E-02	1.176E+01	33	K034	2 2 2 2 2	
7.282E-02	1.254E+01	34	K034	2 2 2 2 2	
6.388E-02	1.100E+01	35	B147	1 2 1 1 2	
7.543E-02	1.299E+01	35	S147	1 2 2 2 2	β form
7.848E-02	1.351E+01	35.5	K034	2 2 2 2 2	
1.259E-01	2.168E+01	37	A028	1 0 2 1 2	intrinsic
7.375E-02	1.270E+01	37	B147	1 2 1 1 2	
8.478E-02	1.460E+01	37	C102	2 0 2 2 2	
8.594E-02	1.480E+01	37	D084	1 0 1 0 2	
8.018E-02	1.381E+01	37	F072	1 0 0 0 2	
8.710E-02	1.500E+01	37	F300	1 0 0 0 1	
8.920E-02	1.536E+01	37	G028	2 2 1 1 2	δ form, recrystallized

(*continued*)

792. $C_6H_8N_2O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.070E-02	1.562E+01	37	G028	2 2 1 1 2	β form, recrystallized
9.120E-02	1.571E+01	37	G028	2 2 1 1 2	α form, recrystallized
9.240E-02	1.591E+01	37	G028	2 2 1 1 2	γ form
8.413E-02	1.449E+01	37	K034	2 2 2 2 2	
8.652E-02	1.490E+01	37	K086	1 0 0 0 2	
8.210E-02	1.414E+01	37	K095	2 0 0 0 2	intrinsic
8.710E-02	1.500E+01	37	L091	1 0 0 0 2	pH 5.5
8.469E-02	1.458E+01	37.50	M142	1 0 0 0 2	
9.201E-02	1.584E+01	39	K034	2 2 2 2 2	
8.362E-02	1.440E+01	40	B147	1 2 1 1 2	form II
9.750E-02	1.679E+01	40	G028	2 2 1 1 2	α form, recrystallized
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	γ form
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	δ form, recrystallized
9.680E-02	1.667E+01	40	G028	2 2 1 1 2	β form, recrystallized
9.518E-02	1.639E+01	40	S147	1 2 2 2 2	β form
1.049E-01	1.807E+01	42	K034	2 2 2 2 2	
1.086E-01	1.870E+01	45	B147	1 2 1 1 2	form II
1.201E-01	2.069E+01	45	S147	1 2 2 2 2	β form
1.256E-01	2.162E+01	46	K034	2 2 2 2 2	
1.527E-01	2.629E+01	50	A047	1 0 0 0 0	EFG
1.388E-01	2.390E+01	50	B147	1 2 1 1 2	form II
1.433E-01	2.468E+01	50	G028	2 2 1 1 2	δ form, recrystallized
1.419E-01	2.444E+01	50	G028	2 2 1 1 2	β form, recrystallized
1.430E-01	2.463E+01	50	G028	2 2 1 1 2	γ form
1.435E-01	2.471E+01	50	G028	2 2 1 1 2	α form, recrystallized
1.516E-01	2.610E+01	50	K034	2 2 2 2 2	
1.488E-01	2.562E+01	50	S147	1 2 2 2 2	β form
1.789E-01	3.080E+01	55	B147	1 2 1 1 2	form II
2.294E-01	3.950E+01	60	B147	1 2 1 1 2	form II
2.923E-01	5.033E+01	65	A047	1 0 0 0 0	EFG
2.962E-01	5.100E+01	65	B147	1 2 1 1 2	form II
3.833E-01	6.600E+01	70	B147	1 2 1 1 2	form II
4.599E-01	7.919E+01	75	A047	1 0 0 0 0	EFG
5.168E-01	8.900E+01	75	B147	1 2 1 1 2	form II
5.660E-01	9.747E+01	79	A047	1 0 0 0 0	EFG
6.272E-02	1.080E+01	ns	D035	0 0 0 0 2	
3.050E-02	5.252E+00	ns	L044	0 0 0 0 2	
4.571E-02	7.871E+00	ns	R427	0 0 0 0 0	
4.365E-02	7.517E+00	ns	R428	0 0 0 0 0	

793. $C_6H_8N_2O_2S.H_2O$
Sulfanilamide (monohydrate)
4-Aminobenzenesulfonamide (monohydrate)
p-Anilinesulfonamide (monohydrate)
Bacteramid (monohydrate)
RN: 20203-81-0 **MP** (°C)**:**
MW: 190.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	4.185E+00	15	G028	2 2 1 1 2	
4.320E-02	8.218E+00	26	G028	2 2 1 1 2	
5.600E-02	1.065E+01	30	G028	2 2 1 1 2	
8.420E-02	1.602E+01	37	G028	2 2 1 1 2	

794. $C_6H_8N_2O_3$
5,5-Dimethylbarbituric acid
5,5-Dimethylbarbitursaeure
Barbituric acid, 5,5-dimethyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-dimethyl
5,5-Dimethyl barbituric acid
5,5-Dimethylbarbiturate
RN: 24448-94-0 **MP** (°C)**:** 278
MW: 156.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.812E-02	2.829E+00	25	P350	0 0 0 0 0	intrinsic
1.549E-02	2.419E+00	ns	T003	0 0 0 0 2	

795. $C_6H_8N_2O_3S$
4-Phenylhydrazine sulfonic acid
Phenylhydrazin-sulfosaeure-(4)
RN: 98-71-5 **MP** (°C)**:**
MW: 188.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.029E-02	5.700E+00	11.50	F300	1 0 0 0 1	
1.860E-01	3.500E+01	100	F300	1 0 0 0 1	

796. $C_6H_8N_2O_8$
Isosorbide dinitrate
1,4:3,6-Dianhydro-D-glucitol dinitrate
Sorbidin
Isogen
Imdur
RN: 87-33-2 **MP** (°C)**:** 70
MW: 236.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-03	5.497E-01	25	L033	1 0 2 1 2	

797. $C_6H_8N_4O$
5-Amino-4-carboxymethylaminopyrimidine
RN: **MP** (°C)**:**
MW: 152.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-01	3.226E+01	100	A082	1 2 0 0 0	

798. $C_6H_8N_8$
2,4,6,7-Tetraminopteridine
2:4:6:7-Tetraminopteridine
RN: 19167-63-6 **MP** (°C)**:**
MW: 192.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.002E-04	7.692E-02	20	A020	1 2 0 1 1	

799. $C_6H_8O_2$
Sorbic acid
2,4-Hexadienoic acid
2-Propenylacrylic acid
Preservastat
Hexadienoic acid
Sorbistat
RN: 110-44-1 **MP** (°C)**:** 134.5
MW: 112.13 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	1.906E+00	30	L069	1 0 1 1 0	EFG

800. $C_6H_8O_6$
Tricarballylic acid
Tricarballylsaeure
1,2,3-Propanetricarboxylic acid
RN: 99-14-9 **MP** (°C)**:** 166
MW: 176.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.885E+00	3.320E+02	18	F300	1 0 0 0 2	

801. $C_6H_8O_6$
Ascorbic acid
L-Ascorbic acid
L-Ascorbinsaeure
RN: 50-81-7 **MP** (°C)**:** 193
MW: 176.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.269E-01	1.633E+02	6.99	A341	0 0 0 0 0	
9.509E-01	1.675E+02	7.99	A341	0 0 0 0 0	
9.880E-01	1.740E+02	9.99	A341	0 0 0 0 0	
1.026E+00	1.807E+02	11.99	A341	0 0 0 0 0	
1.142E+00	2.011E+02	15.99	A341	0 0 0 0 0	
1.418E+00	2.498E+02	20	D041	1 0 0 0 2	
1.254E+00	2.208E+02	20	S472	0 0 0 0 0	
1.283E+00	2.260E+02	20.99	A341	0 0 0 0 0	
1.397E+00	2.460E+02	24.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	25	D315	0 0 0 0 0	
9.757E-01	1.718E+02	25	N003	0 0 0 0 0	
1.388E+00	2.445E+02	25	S472	0 0 0 0 0	
1.551E+00	2.731E+02	28.99	A341	0 0 0 0 0	
1.533E+00	2.699E+02	30	S472	0 0 0 0 0	
1.718E+00	3.025E+02	33.99	A341	0 0 0 0 0	
1.703E+00	2.999E+02	35	S472	0 0 0 0 0	
1.758E+00	3.096E+02	35.99	A341	0 0 0 0 0	
1.856E+00	3.270E+02	38.99	A341	0 0 0 0 0	
1.028E+00	1.810E+02	40	N003	0 0 0 0 0	
1.874E+00	3.301E+02	40	S472	0 0 0 0 0	
2.009E+00	3.539E+02	42.99	A341	0 0 0 0 0	
2.021E+00	3.560E+02	43.99	A341	0 0 0 0 0	
2.066E+00	3.638E+02	44.99	A341	0 0 0 0 0	
2.054E+00	3.618E+02	45	S472	0 0 0 0 0	
2.132E+00	3.755E+02	47.69	A341	0 0 0 0 0	
2.184E+00	3.847E+02	48.49	A341	0 0 0 0 0	
2.235E+00	3.937E+02	49.99	A341	0 0 0 0 0	
2.235E+00	3.936E+02	50	S472	0 0 0 0 0	
2.255E+00	3.972E+02	50.39	A341	0 0 0 0 0	
2.275E+00	4.007E+02	50.99	A341	0 0 0 0 0	
2.373E+00	4.180E+02	52.49	A341	0 0 0 0 0	

(*continued*)

801. $C_6H_8O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.383E+00	4.197E+02	53.99	A341	0 0 0 0 0	
2.413E+00	4.249E+02	54.09	A341	0 0 0 0 0	
2.449E+00	4.314E+02	54.99	A341	0 0 0 0 0	
2.520E+00	4.439E+02	60.02	A341	0 0 0 0 0	
2.551E+00	4.492E+02	61.99	A341	0 0 0 0 0	
2.635E+00	4.641E+02	64.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	ns	M054	0 0 0 0 2	

802. $C_6H_8O_7$

Citric acid anhydrous
2-Hydroxytricarballylic acid
Citronensaeure
1,2,3-Propanetricarboxylic acid
Citro
Citralite

RN: 77-92-9 **MP** (°C)**:** 153
MW: 192.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E+00	4.898E+02	0	M043	1 0 0 0 1	
1.881E+00	3.613E+02	1.2	K084	1 0 1 0 2	
1.875E+00	3.602E+02	1.6	K084	1 0 1 0 2	
2.562E+00	4.923E+02	4.99	A339	0 0 0 0 0	
1.825E+00	3.506E+02	10	D020	1 2 1 1 2	
2.571E+00	4.940E+02	10	F300	1 0 0 0 2	
1.825E+00	3.506E+02	10	F302	1 0 0 0 1	
2.817E+00	5.413E+02	10	M043	1 0 0 0 2	
1.938E+00	3.723E+02	10.0	K084	1 0 1 0 2	
2.684E+00	5.157E+02	9.99	A339	0 0 0 0 0	
1.927E+00	3.702E+02	10.8	K084	1 0 1 0 2	
2.811E+00	5.400E+02	14.99	A339	0 0 0 0 0	
1.933E+00	3.713E+02	15.0	K084	1 0 1 0 2	
2.918E+00	5.605E+02	19.99	A339	0 0 0 0 0	
3.089E+00	5.935E+02	20	D041	1 0 0 0 2	
2.816E+00	5.410E+02	20	F300	1 0 0 0 2	
1.935E+00	3.719E+02	20	F302	1 0 0 0 2	
3.089E+00	5.935E+02	20	M043	1 0 0 0 2	
3.045E+00	5.851E+02	24.99	A339	0 0 0 0 0	
1.994E+00	3.831E+02	25	D020	1 2 1 1 2	
1.254E+01	2.409E+03	25	K040	1 0 2 1 2	
3.201E+00	6.149E+02	29.99	A339	0 0 0 0 0	
2.037E+00	3.914E+02	30	F302	1 0 0 0 2	
3.366E+00	6.466E+02	30	M043	1 0 0 0 2	
3.296E+00	6.332E+02	34.99	A339	0 0 0 0 0	
2.100E+00	4.034E+02	35.8	D039	2 2 1 2 2	EFG
2.094E+00	4.023E+02	36.6	F302	1 0 0 0 2	
3.201E+00	6.150E+02	36.60	F300	1 0 0 0 2	

(*continued*)

802. $C_6H_8O_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.346E+00	6.429E+02	39.99	A339	0 0 0 0 0	
2.118E+00	4.069E+02	40	D020	1 2 1 1 2	
2.116E+00	4.065E+02	40	D039	2 2 1 2 0	EFG
2.118E+00	4.069E+02	40	F302	1 0 0 0 2	
3.553E+00	6.825E+02	40	M043	1 0 0 0 2	
3.438E+00	6.605E+02	44.99	A339	0 0 0 0 0	
3.488E+00	6.702E+02	49.99	A339	0 0 0 0 0	
2.161E+00	4.152E+02	50	D039	2 2 1 2 0	EFG
2.159E+00	4.149E+02	50	F302	1 0 0 0 2	
3.539E+00	6.800E+02	54.99	A339	0 0 0 0 0	
3.601E+00	6.918E+02	59.99	A339	0 0 0 0 0	
2.214E+00	4.253E+02	60	D039	2 2 1 2 0	EFG
2.205E+00	4.236E+02	60	F302	1 0 0 0 2	
3.824E+00	7.347E+02	60	M043	1 0 0 0 2	
3.669E+00	7.050E+02	64.99	A339	0 0 0 0 0	
2.261E+00	4.344E+02	70	D039	2 2 1 2 0	EFG
2.251E+00	4.325E+02	70	F302	1 0 0 0 2	
2.300E+00	4.420E+02	80	D039	2 2 1 2 0	EFG
2.294E+00	4.407E+02	80	F302	1 0 0 0 2	
4.102E+00	7.881E+02	80	M043	1 0 0 0 2	
2.350E+00	4.515E+02	90	D039	2 2 1 2 0	EFG
2.336E+00	4.487E+02	90	F302	1 0 0 0 2	
2.391E+00	4.595E+02	100	D039	2 2 1 2 0	EFG
4.372E+00	8.400E+02	100	D041	1 0 0 0 2	
3.997E+00	7.680E+02	100	F300	1 0 0 0 2	
2.376E+00	4.565E+02	100	F302	1 0 0 0 1	
4.373E+00	8.403E+02	100	M043	1 0 0 0 2	
1.885E+00	3.621E+02	.0	K084	1 0 1 0 2	

803. $C_6H_8O_7.H_2O$

Citric acid (monohydrate)
2-Hydroxytricarballylic acid (monohydrate)
RN: 5949-29-1 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E+00	3.266E+02	0	D039	2 2 1 2 0	EFG
1.667E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
3.005E+00	6.314E+02	17.20	L031	1 1 2 1 2	average of 2
3.077E+00	6.466E+02	19.80	L031	1 1 2 1 2	
1.771E+00	3.723E+02	20	D039	2 2 1 2 0	EFG
3.080E+00	6.473E+02	20.20	L031	1 1 2 1 2	
3.146E+00	6.610E+02	22.50	L031	1 1 2 1 2	
3.154E+00	6.627E+02	22.90	L031	1 1 2 1 2	
1.822E+00	3.830E+02	25	D039	2 2 1 2 2	EFG
3.214E+00	6.753E+02	25.10	L031	1 1 2 1 2	
3.216E+00	6.759E+02	25.30	L031	1 1 2 1 2	

(*continued*)

803. $C_6H_8O_7.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.272E+00	6.875E+02	27.00	L031	1 1 2 1 2	
3.276E+00	6.885E+02	27.60	L031	1 1 2 1 2	
3.303E+00	6.942E+02	28.60	L031	1 1 2 1 2	
1.864E+00	3.917E+02	30	D039	2 2 1 2 0	EFG
3.359E+00	7.059E+02	30.50	L031	1 1 2 1 2	
3.357E+00	7.054E+02	30.70	L031	1 1 2 1 2	
3.389E+00	7.122E+02	31.80	L031	1 1 2 1 2	
3.440E+00	7.230E+02	33.70	L031	1 1 2 1 2	
3.478E+00	7.308E+02	34.40	L031	1 1 2 1 2	
3.518E+00	7.392E+02	35.40	L031	1 1 2 1 2	

804. C_6H_8S

2-Ethylthiophene

Thiophene, 2-ethyl-

RN: 872-55-9 **MP** (°C)**:** <25

MW: 112.19 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.603E-03	2.920E-01	25	K119	1 0 0 0 2	
2.603E-03	2.920E-01	25	P051	2 1 1 2 2	
2.603E-03	2.920E-01	25.00	P007	2 1 2 2 2	

805. $C_6H_9ClO_3$

Ethyl 2-chloroacetoacetate

2-Chloroacetoacetic acid ethyl ester

RN: 609-15-4 **MP** (°C)**:**

MW: 164.59 **BP** (°C)**:** 107 at 14 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-02	8.900E+00	30	B433	0 0 0 0 0	

806. $C_6H_9NO_3$

4,6,10-Trioxa-1-azatricyclo[3.3.1.13,7]decane

Trimorpholin

Trimorpholine

RN: 281-36-7 **MP** (°C)**:**

MW: 143.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	1.670E+02	0	F300	1 0 0 0 2	
2.375E+00	3.400E+02	80	F300	1 0 0 0 2	

807. $C_6H_9NO_3$
Trimethadione
3,5,5-Trimethyl-2,4-diketooxazolidine
3,5,5-Trimethyl-2,4-oxazolidinedione
Tridione
RN: 127-48-0 **MP** (°C)**:** 46
MW: 143.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-01	4.762E+01	20	D041	1 0 0 0 0	

808. $C_6H_9NO_6$
Triglycine
Complexon I
N,N-bis(Carboxymethyl)glycine
α,α′,α²-Trimethylaminetricarboxylic acid
RN: 139-13-9 **MP** (°C)**:** 241.5
MW: 191.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-01	5.906E+01	25	M024	1 2 0 1 2	
3.395E-01	6.490E+01	25.1	N024	0 0 0 0 0	
3.374E-01	6.450E+01	25.1	N025	0 0 0 0 0	
3.348E-01	6.400E+01	25.1	N026	0 0 0 0 0	
3.101E-01	5.927E+01	25.1	N027	1 2 2 2 2	

809. $C_6H_9N_3$
Kyanmethin
6-Amino-2,4-dimethyl-pyrimidin
6-Amino-2,4-dimethylpyrimidine
RN: 461-98-3 **MP** (°C)**:** 182
MW: 123.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.197E-02	6.400E+00	18	F300	1 0 0 0 1	

810. $C_6H_9N_3O_2$
2-Isopropyl-4(5)-nitroimidazole
1H-Imidazole, 2-(1-methylethyl)-4-nitro-
2-(1-Methylethyl)-4-nitro-1H-imidazole
2-Isopropyl-5-nitroimidazole
2-Isopropyl-4-nitroimidazole
RN: 13373-32-5 **MP** (°C)**:** 182–183
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
6.886E-02	1.068E+01	20	D344	0 0 0 0 0	
7.030E-02	1.091E+01	20	D344	0 0 0 0 0	

811. $C_6H_9N_3O_2$
L-Histidine
L-Histidin
Histidine
RN: 71-00-1 **MP** (°C)**:** 287
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.580E-01	4.003E+01	15	D349	2 1 1 2 2	
2.646E-01	4.106E+01	20	B032	1 2 2 1 2	
2.640E-01	4.096E+01	20	D349	2 1 1 2 2	
2.930E-01	4.546E+01	25	B032	1 2 2 1 2	
2.574E-01	3.994E+01	25	D041	1 0 0 0 2	
2.720E-01	4.220E+01	25	D349	2 1 1 2 2	
2.481E-01	3.850E+01	25	F300	1 0 0 0 2	
2.651E-01	4.114E+01	25	G315	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N024	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N025	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N026	0 0 0 0 0	
2.675E-01	4.150E+01	25.1	N027	1 1 2 2 2	
2.791E-01	4.330E+01	27	D036	0 0 0 0 0	
3.207E-01	4.976E+01	29.80	B032	1 2 2 1 2	
2.834E-01	4.398E+01	30	H062	2 2 2 0 1	EFG
5.213E-01	8.088E+01	50	H062	2 2 2 0 0	EFG
7.915E-01	1.228E+02	70	H062	2 2 2 0 0	EFG

812. $C_6H_9N_3O_2$
6-Amino-1,3-dimethyluracil
RN: 6642-31-5 **MP** (°C)**:**
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.550E-02	7.060E+00	25	Z408	0 0 0 0 0	

813. $C_6H_9N_3O_3$
Metronidazole
Flagyl
2-Methyl-5-nitroimidazole-1-ethanol
Metrozine
Rozex
2-Methyl-5-nitro-1-imidazoleethanol
RN: 443-48-1 **MP** (°C)**:** 158
MW: 171.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.441E-02	9.312E+00	20	D344	0 0 0 0 0	
5.540E-02	9.482E+00	20	D344	0 0 0 0 0	
4.809E-02	8.232E+00	20	H324	0 0 0 0 0	
5.785E-02	9.901E+00	20	I315	0 0 0 0 0	
6.427E-02	1.100E+01	25	C062	1 1 2 1 2	
5.550E-02	9.500E+00	25	C124	2 0 1 1 2	
5.727E-02	9.803E+00	26	H324	0 0 0 0 0	
6.585E-02	1.127E+01	30	H324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	C324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	K444	0 0 0 0 0	

814. C_6H_{10}
1,5-Hexadiene
Biallyl
Diallyl
RN: 592-42-7 **MP** (°C)**:** –141
MW: 82.15 **BP** (°C)**:** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.057E-03	1.690E-01	25	M001	2 1 2 2 2	

815. C_6H_{10}
Cyclohexene
1,2,3,4-Tetrahydrobenzene
RN: 110-83-8 **MP** (°C)**:** –104
MW: 82.15 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-03	2.799E-01	4.8	L007	2 2 1 2 2	
3.408E-03	2.799E-01	5.1	L007	2 0 1 1 2	
3.633E-03	2.984E-01	14.8	L007	2 2 1 2 2	
3.633E-03	2.984E-01	15.2	L007	2 0 1 1 2	
1.583E-03	1.300E-01	20	C008	1 2 2 0 1	
2.769E-03	2.274E-01	20	M337	2 1 2 2 2	

(*continued*)

815. C_6H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-03	2.834E-01	23.5	S171	2 1 2 2 2	
3.639E-03	2.989E-01	24.8	L007	2 2 1 2 2	
2.593E-03	2.130E-01	25	M001	2 1 2 2 2	
3.639E-03	2.989E-01	25.1	L007	2 0 1 1 2	
3.681E-03	3.024E-01	34.8	L007	2 2 1 2 2	
3.681E-03	3.024E-01	35.2	L007	2 0 1 1 2	
6.000E-03	4.929E-01	40	P335	0 0 0 0 0	
3.779E-03	3.104E-01	44.8	L007	2 2 1 2 2	
3.779E-03	3.104E-01	45.2	L007	2 0 1 1 2	
1.800E-02	1.479E+00	140	P335	0 0 0 0 0	
1.583E-03	1.300E-01	ns	M010	0 0 0 0 1	

816. C_6H_{10}

1-Hexyne
Butylacetylene
n-Butylacetylene

RN: 693-02-7 **MP** (°C)**:** –132
MW: 82.15 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.382E-03	3.600E-01	25	M001	2 1 2 2 2	
8.370E-03	6.876E-01	25	M342	1 0 1 1 2	

817. C_6H_{10}

3-Hexyne
Diethylacetylene

RN: 928-49-4 **MP** (°C)**:** –103
MW: 82.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	5.586E-01	25	H039	1 2 2 2 1	
6.400E-03	5.257E-01	35	H039	1 2 2 2 1	

818. $C_6H_{10}BrNO_4$

5-Bromo-2-ethyl-5-nitro-1,3-dioxane
2-Ethyl-5-bromo-5-nitro-1,3-dioxane

RN: 54010-85-4 **MP** (°C)**:** 58–59
MW: 240.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.205E-03	7.694E-01	25	L013	1 0 2 1 2	

819. $C_6H_{10}BrNO_4$

5-Bromo-2,2-dimethyl-5-nitro-1,3-dioxane
2,2-Dimethyl-5-bromo-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-2,2-dimethyl-5-nitro-
RN: 60766-57-6 **MP** (°C)**:** 79–81
MW: 240.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.369E-03	1.049E+00	25	L013	1 0 2 1 2	

820. $C_6H_{10}ClN_5$

Deethylatrazine
2-Amino-4-isopropylamino-6-chloro-*s*-triazine
6-Chloro-*N*-(1-methylethyl)-1,3,5-triazine-2,4-diamine
RN: 6190-65-4 **MP** (°C)**:**
MW: 187.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.753E-01	2	B193	1 1 0 0 1	

821. $C_6H_{10}O$

Mesityl oxide
Mesityloxid
RN: 141-79-7 **MP** (°C)**:** –57
MW: 98.15 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.862E-01	2.809E+01	20	D052	1 1 0 0 0	
2.975E-01	2.920E+01	ns	F300	0 0 0 0 2	

822. $C_6H_{10}O$

Cyclohexanone
Cyclohexanon
RN: 108-94-1 **MP** (°C)**:** –47
MW: 98.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-02	1.298E+00	20	D052	1 1 0 0 1	*sic*
2.485E-01	2.439E+01	25	B060	2 0 1 1 1	
8.975E-01	8.809E+01	25	M323	2 2 1 1 2	

823. $C_6H_{10}OS_2$

Allicin
2-Propene-1-sulfinothioic acid *S*-2-propenyl ester
RN: 539-86-6 **MP** (°C)**:** <25
MW: 162.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-01	2.400E+01	10	F300	1 0 0 0 1	

824. $C_6H_{10}O_2$

Methyl vinyl carbinol acetate
1-Methylallyl acetate
3-Buten-2-yl acetate
RN: 6737-11-7 **MP** (°C)**:**
MW: 114.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-01	1.303E+01	26	O012	1 2 1 1 2	
6.953E-02	7.937E+00	50	O012	1 2 1 1 2	
1.718E-01	1.961E+01	75	O012	1 2 1 1 2	

825. $C_6H_{10}O_2$

3-Methyl-1,3-pentadione
1,2-Dimethyl-1,3-butadiene
3,4-Dimethylbutadiene
RN: 4549-74-0 **MP** (°C)**:** –5
MW: 114.15 **BP** (°C)**:** 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.780E-01	1.116E+02	25	M078	2 0 1 0 2	

826. $C_6H_{10}O_2S_4$

Dixanthogen
Ethyl dixanthogen
RN: 502-55-6 **MP** (°C)**:** 28
MW: 242.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.151E-03	22	P076	1 2 1 1 1	
1.140E-05	2.763E-03	25	H102	1 2 1 2 2	
<2.06E-06	<5.00E-04	25	M161	1 0 0 0 0	
1.250E-05	3.030E-03	ns	L083	0 0 0 0 0	EFG, pH 3–9

827. $C_6H_{10}O_3$
Ethyl acetoacetate
Acetessigsaeure-aethyl ester
Acetoacetic acid ethyl ester
RN: 141-97-9 **MP** (°C)**:** –45
MW: 130.14 **BP** (°C)**:** 180.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.613E-01	1.251E+02	10.5	D041	1 0 0 0 2	
8.529E-01	1.110E+02	16.50	F300	1 0 0 0 2	

828. $C_6H_{10}O_4$
2,2-Dimethylsuccinic acid
α,α-Dimethylbernsteinsaeure
RN: 597-43-3 **MP** (°C)**:** 140.5
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.790E-01	7.000E+01	14	F300	1 0 0 0 2	

829. $C_6H_{10}O_4$
sym-Dimethylsuccinic acid
Acide Dimethylsuccinique-*sym*
RN: 608-40-2 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	3.000E+02	15	M051	1 0 0 0 2	

830. $C_6H_{10}O_4$
n-Propylmalonic acid
Acide *n*-propylmalonique
RN: 616-62-6 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E+00	4.560E+02	0	M051	1 0 0 0 2	
4.112E+00	6.010E+02	15	M051	1 0 0 0 2	
4.790E+00	7.000E+02	25	M051	1 0 0 0 2	
6.459E+00	9.440E+02	50	M051	1 0 0 0 2	

831. $C_6H_{10}O_4$
Ethylene glycol diacetate
Glycol diacetate
RN: 111-55-7 **MP** (°C)**:** –31
MW: 146.14 **BP** (°C)**:** 190

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.756E+02	20	D052	1 1 0 0 2	
9.661E-01	1.412E+02	20	M062	1 0 0 0 2	
8.526E-01	1.246E+02	22	F300	1 0 0 0 2	
1.034E+00	1.511E+02	24.50	O005	2 0 2 2 2	
1.070E+00	1.564E+02	25	F064	1 0 0 0 2	
1.220E-01	1.783E+01	ns	F014	0 0 0 0 2	

832. $C_6H_{10}O_4$
DL-2,3-Dimethylsuccinic acid
DL-α,α′-Dimethylbernsteinsaeure
RN: 13545-04-5 **MP** (°C)**:** 120
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-01	3.000E+01	14	F300	1 0 0 0 0	

833. $C_6H_{10}O_4$
Adipic acid
Adipinsaeure
RN: 124-04-9 **MP** (°C)**:** 152
MW: 146.14 **BP** (°C)**:** 337.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.431E-02	7.937E+00	0	M043	1 0 0 0 0	
6.766E-02	9.888E+00	4.99	A339	0 0 0 0 0	
6.775E-02	9.901E+00	10	M043	1 0 0 0 1	
7.853E-02	1.148E+01	9.99	A339	0 0 0 0 0	
1.061E-01	1.551E+01	14.99	A339	0 0 0 0 0	
9.580E-02	1.400E+01	15	F300	1 0 0 0 1	
9.580E-02	1.400E+01	15	L041	1 0 0 1 1	
9.580E-02	1.400E+01	15	M051	1 0 0 0 1	
1.303E-01	1.904E+01	19.99	A339	0 0 0 0 0	
1.011E-01	1.478E+01	20	D041	1 0 0 0 1	
1.276E-01	1.865E+01	20	M043	1 0 0 0 1	
9.856E-02	1.440E+01	20	M171	1 0 0 0 1	
9.000E-02	1.315E+01	20	S006	1 0 0 0 1	
4.824E-01	7.050E+01	21	B040	1 0 1 1 2	*sic*
1.664E-01	2.432E+01	24.99	A339	0 0 0 0 0	
2.216E-03	3.239E-01	25	K035	2 0 0 0 2	*sic*
2.053E-01	3.001E+01	29.99	A339	0 0 0 0 0	

(*continued*)

833. $C_6H_{10}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-01	2.913E+01	30	M043	1 0 0 0 1	
2.045E-01	2.988E+01	34.10	A031	1 2 2 2 2	
2.546E-01	3.721E+01	34.99	A339	0 0 0 0 0	
2.933E-01	4.287E+01	39.3	G302	2 2 2 2 0	EFG
3.274E-01	4.785E+01	39.99	A339	0 0 0 0 0	
3.333E-01	4.871E+01	40	A031	1 2 2 2 2	
3.382E-01	4.943E+01	40	B088	1 0 0 0 1	
3.258E-01	4.762E+01	40	M043	1 0 0 0 1	
4.383E-01	6.406E+01	44.99	A339	0 0 0 0 0	
5.516E-01	8.062E+01	49.99	A339	0 0 0 0 0	
5.788E-01	8.458E+01	50	A031	1 2 2 2 2	
7.508E-01	1.097E+02	54.99	A339	0 0 0 0 0	
1.011E+00	1.477E+02	59.99	A339	0 0 0 0 0	
1.024E+00	1.497E+02	60	A031	1 2 2 2 2	
1.044E+00	1.525E+02	60	M043	1 0 0 0 1	
1.130E+00	1.652E+02	64.99	A339	0 0 0 0 0	
1.740E+00	2.543E+02	70	A031	1 2 2 2 2	
2.818E+00	4.118E+02	80	M043	1 0 0 0 1	
3.330E+00	4.867E+02	87.10	A031	1 2 2 2 2	
4.277E+00	6.250E+02	100	F300	1 0 0 0 2	
4.211E+00	6.154E+02	100	M043	1 0 0 0 2	
1.662E-01	2.430E+01	rt	H431	0 0 0 0 0	

834. $C_6H_{10}O_4$

Methyl α-acetoxypropionate
Methyl 2-acetoxypropionate
Methyl *O*-acetyllactate
Methyl 2-acetyloxypropanoate

RN: 6284-75-9 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-01	8.120E+01	25	R006	2 2 0 1 2	

835. $C_6H_{10}O_5$

Propanoic acid, 2-[(methoxycarbonyl)oxy]-, methyl ester
Carbonic acid, methyl ester, ester with methyl lactate

RN: 6288-11-5 **MP** (°C)**:**
MW: 162.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-01	3.911E+01	25	R007	0 0 0 0 0	

836. $C_6H_{10}O_8$
D-Talogalactaric acid
D-Taloschleimsaeure
D-Galactaric acid
Galactaric acid
Schleimsaeure
RN: 526-99-8 **MP** (°C)**:** > 230
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	3.289E+00	14	D041	1 0 0 0 1	
1.570E-02	3.300E+00	14	F300	1 0 0 0 1	
8.090E-02	1.700E+01	100	F300	1 0 0 0 1	

837. $C_6H_{11}Br$
Bromocyclohexane
Cyclohexyl bromide
RN: 108-85-0 **MP** (°C)**:**
MW: 163.06 **BP** (°C)**:** 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.012E-03	8.173E-01	ns	S460	0 0 0 0 0	

838. $C_6H_{11}BrN_2O_2$
α-Methyl-γ-bromo-butanoic ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.658E-02	1.039E+01	ns	F056	0 2 2 2 1	

839. $C_6H_{11}BrN_2O_2$
α-Bromo-isovaleric ureide
Butanamide, *N*-(aminocarbonyl)-2-bromo-3-methyl-
Dormigene
Pivadorn
Pivadorm
Isobromyl
RN: 496-67-3 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.531E-02	1.903E+01	ns	F057	0 2 2 2 2	

840. $C_6H_{11}BrN_2O_2$
3-Bromo-2-methyl-butanoic ureide
Urea, (2-bromo-2-methylbutyryl)-
DL-*N*-(2-Bromo-2-methylbutanoyl)urea
RN: 14368-76-4 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	3.101E+01	ns	F056	0 2 2 2 1	

841. $C_6H_{11}BrN_2O_2$
β-Bromo-valeric acid ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.470E-02	7.740E+00	ns	F056	0 2 2 2 1	

842. $C_6H_{11}BrN_2O_2$
γ-Bromo-valeric acid ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.307E-02	9.607E+00	ns	F056	0 2 2 2 1	

843. $C_6H_{11}BrN_2O_2$
α-Bromo-valeric acid ureide
Pentanamide, *N*-(aminocarbonyl)-2-bromo-
RN: 66947-87-3 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-02	8.232E+00	ns	F056	0 2 2 2 1	
3.703E-02	8.261E+00	ns	F057	0 2 2 2 2	

844. $C_6H_{11}NO$
Caprolactam
ε-Caprolactam
RN: 105-60-2 **MP** (°C)**:** 70
MW: 113.16 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.776E+00	4.273E+02	5.70	B201	2 2 2 1 2	
3.850E+00	4.357E+02	10.30	B201	2 2 2 1 2	

845. $C_6H_{11}NO$

Cyclohexanone oxime
Antioxidant D
(Hydroxyimino)cyclohexane

RN: 100-64-1 **MP** (°C)**:** 90
MW: 113.16 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.409E-01	1.594E+01	25.5	K087	1 0 0 0 2	
1.580E-01	1.787E+01	32.0	K087	1 0 0 0 2	
1.648E-01	1.865E+01	36.8	K087	1 0 0 0 2	
1.936E-01	2.191E+01	44.0	K087	1 0 0 0 2	
2.155E-01	2.439E+01	48.8	K087	1 0 0 0 2	
2.715E-01	3.073E+01	60.4	K087	1 0 0 0 2	
2.922E-01	3.307E+01	63.7	K087	1 0 0 0 2	
3.194E-01	3.614E+01	76.2	K087	1 0 0 0 2	
3.456E-01	3.911E+01	83.1	K087	1 0 0 0 2	
4.039E-01	4.571E+01	95.2	K087	1 0 0 0 2	
4.939E-01	5.589E+01	110.7	K087	1 0 0 0 2	
5.743E-01	6.498E+01	120	K087	1 0 0 0 2	
7.386E-01	8.358E+01	131	K087	1 0 0 0 2	

846. $C_6H_{11}NO_2S$

2,2-Dimethylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2,2-dimethyl-
Thiazolidine-4-carboxylic acid, 2,2-dimethyl-

RN: 42607-20-5 **MP** (°C)**:**
MW: 161.22 **BP** (°C)**:** 317.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	4.837E+01	21	B414	1 0 0 1 1	very fast and extent decompostion, uncertain value

847. $C_6H_{11}NO_4$

α-Aminoadipic acid
2-Aminohexanedioic acid
α-Amino-adipinsaeure

RN: 542-32-5 **MP** (°C)**:**
MW: 161.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.365E-02	2.200E+00	20	F300	1 0 0 0 1	

848. $C_6H_{11}NO_4$
Glycine, *N*-(carboxymethyl)-, 1-ethyl ester
AcGlyOEt
Acetic acid, iminodi-, monoethyl ester
RN: 21885-31-4 **MP** (°C)**:**
MW: 161.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.074E-03	1.140E+00	27	D036	0 0 0 0 0	

849. $C_6H_{11}N_2O_4PS_3$
Methidathion
Supracide
S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl) *O,O*-dimethyl phosphorodithioate
Ultracide
Somanil
S-2,3-Dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl *O,O*-dimethylphosphorodithioate
RN: 950-37-8 **MP** (°C)**:**
MW: 302.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.186E-04	1.870E-01	20	B300	2 2 1 1 2	
8.269E-04	2.500E-01	20	F311	1 2 2 2 1	
7.938E-04	2.400E-01	25	M161	1 0 0 0 2	

850. $C_6H_{11}N_3O_6$
Glycine tripeptide
RN: **MP** (°C)**:**
MW: 221.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.127E-01	4.705E+01	20	B032	1 2 2 1 2	
2.907E-01	6.430E+01	25	B032	1 2 2 1 2	
3.565E-01	7.884E+01	29.80	B032	1 2 2 1 2	

851. C_6H_{12}
Methylcyclopentane
MCP
RN: 96-37-7 **MP** (°C)**:** –142
MW: 84.16 **BP** (°C)**:** 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	K119	1 0 0 0 2	
4.990E-04	4.200E-02	25	M001	2 1 2 2 2	
5.062E-04	4.260E-02	25	M002	2 1 2 2 2	

(*continued*)

851. C_6H_{12} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	P051	2 1 1 2 2	
4.967E-04	4.180E-02	25.00	P007	2 1 2 2 2	
4.990E-04	4.200E-02	ns	H123	0 0 0 0 0	

852. C_6H_{12}

Cyclohexane
Cyclohexan

RN: 110-82-7 **MP** (°C)**:** 7
MW: 84.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.734E-04	8.192E-02	4.8	L007	2 1 1 2 2	
9.734E-04	8.192E-02	5.1	L007	2 0 1 1 2	
1.054E-03	8.869E-02	14.8	L007	2 1 1 2 2	
1.054E-03	8.869E-02	15.2	L007	2 0 1 1 2	
9.505E-04	8.000E-02	16	D047	1 0 0 1 1	
<5.94E-04	<5.00E-02	17	F300	1 0 0 0 0	
4.396E-04	3.700E-02	20	M337	2 1 2 2 2	
6.178E-04	5.200E-02	23.5	S171	2 1 2 2 2	
1.055E-03	8.883E-02	24.8	L007	2 1 1 2 2	
9.505E-04	7.999E-02	25	G068	1 0 1 0 0	
6.939E-04	5.840E-02	25	G313	2 1 1 2 2	
1.426E-03	1.200E-01	25	K112	1 0 2 1 1	
7.901E-04	6.650E-02	25	K119	1 0 0 0 2	
6.737E-04	5.670E-02	25	L002	2 2 2 2 2	
6.535E-04	5.500E-02	25	M001	2 1 2 2 2	
6.535E-04	5.500E-02	25	M002	2 1 2 2 2	
6.535E-04	5.500E-02	25	M040	1 0 0 1 1	
6.832E-04	5.750E-02	25	M132	2 2 2 1 2	
7.901E-04	6.650E-02	25	P051	2 1 1 2 2	
6.270E-04	5.277E-02	25	S359	2 1 2 2 2	
7.901E-04	6.650E-02	25.00	P007	2 1 2 2 2	
1.055E-03	8.883E-02	34.8	L007	2 1 1 2 2	
1.055E-03	8.883E-02	35.2	L007	2 0 1 1 2	
5.389E-04	4.535E-02	38	K055	1 2 0 1 1	
1.085E-03	9.131E-02	44.8	L007	2 1 1 2 2	
1.085E-03	9.131E-02	45.2	L007	2 0 1 1 2	
1.426E-03	1.200E-01	50	L097	1 1 1 1 1	
2.020E-03	1.700E-01	56	G068	1 0 1 0 1	
3.222E-04	2.712E-02	71	K055	1 2 0 1 1	
3.326E-03	2.799E-01	94	G068	1 0 1 0 1	
1.200E-04	1.010E-02	ns	D348	0 0 0 0 0	
6.535E-04	5.500E-02	ns	H123	0 0 0 0 0	
5.000E-03	4.208E-01	ns	H333	0 1 0 1 0	EFG
9.505E-04	8.000E-02	ns	M010	0 0 0 0 0	
6.642E-04	5.590E-02	ns	M175	0 0 2 1 2	

853. C_6H_{12}
4-Methyl-1-pentene
4-Methylpentene
Isohexene
RN: 691-37-2 **MP** (°C)**:** –154
MW: 84.16 **BP** (°C)**:** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.703E-04	4.800E-02	25	M001	2 1 2 2 1	

854. C_6H_{12}
2-Methyl-1-pentene
4-Methyl-4-pentene
RN: 763-29-1 **MP** (°C)**:** –136
MW: 84.16 **BP** (°C)**:** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.268E-04	7.800E-02	25	M001	2 1 2 2 2	

855. C_6H_{12}
1-Hexene
1-*n*-Hexene
Hexene
Dialen 6
RN: 592-41-6 **MP** (°C)**:** –140
MW: 84.16 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.822E-04	4.900E-02	23	C332	0 0 0 0 0	
6.583E-04	5.540E-02	25	L002	2 2 2 2 2	
5.941E-04	5.000E-02	25	M001	2 1 2 2 2	
5.941E-04	5.000E-02	25	M040	1 0 0 1 1	
8.280E-04	6.969E-02	25	M342	1 0 1 1 2	

856. $C_6H_{12}ClNO$
Acetamide, 2-chloro-*N*,*N*-diethyl-
CDEA
RN: 2315-36-8 **MP** (°C)**:**
MW: 149.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.264E-01	7.877E+01	25	B185	0 0 0 0 0	

857. $C_6H_{12}Cl_2O$
Dichloroisopropyl ether
bis(2-Chloro-1-methylethyl) ether
DCIP
β,β′-Dichlorodiisopropyl ether
2,2′-Oxybis[1-chloropropane]
Pichloram
RN: 63283-80-7 **MP** (°C)**:**
MW: 171.07 **BP** (°C)**:** 187.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.921E-03	1.697E+00	20	M062	1 0 0 0 1	

858. $C_6H_{12}Cl_2O_2$
1,2-bis(2-Chloroethoxy)ethane
Triglycol dichloride
RN: 112-26-5 **MP** (°C)**:** 121
MW: 187.07 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.916E-02	1.855E+01	20	M062	1 0 0 0 2	

859. $C_6H_{12}Cl_3O_4P$
tris-(2-Chloroethyl) phosphate
Tri-β-chloroethyl phosphate
RN: 115-96-8 **MP** (°C)**:**
MW: 285.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.01E-04	<2.00E-01	25	B070	1 2 0 1 0	

860. $C_6H_{12}NO_3PS_2$
Diethyl 1,3-dithietan-2-ylidenephosphoramidate
Nematak
AC 64475
Geofos
Fosthietan
CL 64475
RN: 21548-32-3 **MP** (°C)**:**
MW: 241.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.072E-01	5.000E+01	25	M161	1 0 0 0 1	

861. $C_6H_{12}NO_4PS_2$
Formothion
O,*O*-Dimethyl *S*-(*N*-methyl-*N*-formylcarbamoylmethyl) dithiophosphate
RN: 2540-82-1 **MP** (°C)**:**
MW: 257.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-02	2.600E+00	24	M161	1 0 0 0 1	

862. $C_6H_{12}N_2O$
N-Nitrosohexamethyleneimine
NHMI
RN: 932-83-2 **MP** (°C)**:**
MW: 128.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.282E+01	24	M031	1 1 1 1 1	

863. $C_6H_{12}N_2O_2$
2,6-Dimethylnitrosomorpholine
DMNM
RN: 1456-28-6 **MP** (°C)**:**
MW: 144.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-01	1.240E+02	24	M031	1 1 1 1 1	

864. $C_6H_{12}N_2O_2$
Adipamide
Adipinsaeurediamid
RN: 628-94-4 **MP** (°C)**:**
MW: 144.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.052E-02	4.400E+00	12.20	F300	1 0 0 0 1	

865. $C_6H_{12}N_2O_3$
Daminozide
N-Dimethylamino-β-carbamyl propionic acid
Succinic acid 2,2-dimethylhydrazide
Alar
DMASA
RN: 1596-84-5 **MP** (°C)**:** 155
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-01	1.000E+02	25	M161	1 0 0 0 2	

866. $C_6H_{12}N_2O_3$
δ-Aminovaleric hydantoic acid
δ-Uramidovaleric acid
RN: **MP** (°C)**:** 179
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.740E-02	2.787E+00	25	M024	1 2 0 1 2	

867. $C_6H_{12}N_2O_3S$
Methomyl
Acetamidic acid
N-[(methyl-carbamoyl)oxy]-, methyl ester
Carbamic acid
Lannabait
Nudrin
RN: 16752-77-5 **MP** (°C)**:** 78
MW: 192.24 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.548E-01	6.821E+01	ns	R424	0 0 0 0 0	

868. $C_6H_{12}N_2O_4S_2$
L-Cystine
3,3′-Dithiobis(2-aminopropanoic acid)
RN: 56-89-3 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.021E-03	4.858E-01	20	H082	1 2 1 1 2	isomeric
7.905E-04	1.900E-01	20	H082	1 2 1 1 2	plate cystine
6.910E-04	1.660E-01	24.99	C404	2 1 2 2 1	
7.000E-02	1.682E+01	25	C405	2 1 2 2 2	intrinsic zwit

(*continued*)

868. $C_6H_{12}N_2O_4S_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-04	1.090E-01	25	D017	1 0 0 0 2	
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.661E-04	1.120E-01	25	L001	1 0 1 1 2	pH 6.0
4.910E-04	1.180E-01	27	D036	0 0 0 0 0	
7.100E-04	1.706E-01	34.99	C404	2 1 2 2 1	
8.500E-04	2.043E-01	44.99	C404	2 1 2 2 1	
2.163E-03	5.197E-01	75	D041	1 0 0 0 1	
4.536E-04	1.090E-01	rt	B103	0 0 0 0 2	

869. $C_6H_{12}N_2O_4S$

DL-Lanthionine

L-Cysteine, *S*-[(2*R*)-2-amino-2-carboxyethyl]-

RN: 922-55-4 **MP** (°C)**:** 280

MW: 208.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.193E-03	1.498E+00	25	D041	1 0 0 0 1	

870. $C_6H_{12}N_2O_4S_2$

Mesocystine

meso-Cystine

RN: 6020-39-9 **MP** (°C)**:**

MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	5.600E-02	25	L001	1 0 1 1 1	pH 6.0

871. $C_6H_{12}N_2O_4S_2$

D-Cystine

D-(+)-3,3′-Dithiobis(2-aminopropanoic acid)

RN: 349-46-2 **MP** (°C)**:** 227

MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.702E-04	1.130E-01	25	L001	1 0 1 1 2	pH 6.0

872. $C_6H_{12}N_2O_4S_2$
DL-Cystine
Cystine
RN: 923-32-0 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-04	4.900E-02	25	D041	1 0 0 0 1	
2.372E-04	5.700E-02	25	L001	1 0 1 1 1	pH 6.0

873. $C_6H_{12}N_2S_4$
Thiram
Tetramethylthioperoxydicarbonothioic diamine
Tetramethylthiuram disulfide
N,*N*′-(Dithiodicarbonothioyl)bis(*N*-methylmethanamine)
Arasan
Nomersan
RN: 137-26-8 **MP** (°C)**:** 155.5
MW: 240.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.413E-05	1.782E-02	ns	R427	0 0 0 0 0	
1.248E-04	3.000E-02	rt	M161	0 0 0 0 1	

874. $C_6H_{12}N_2S_4Zn$
Ziram
Zinc *bis* dimethyldithiocarbamate
Corozate
Karbam white
Fuklasin
Fuclasin
RN: 137-30-4 **MP** (°C)**:** 240
MW: 305.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-04	6.500E-02	20	F300	1 0 0 0 1	
1.308E-05	4.000E-03	20	F311	1 2 2 2 1	*sic*
2.125E-04	6.500E-02	25	M161	1 0 0 0 1	

875. $C_6H_{12}N_4$
Methenamine
Hexamethylen-tetramin
RN: 100-97-0 **MP** (°C)**:**
MW: 140.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.231E+00	3.128E+02	1.99	B442	0 0 0 0 0	
2.202E+00	3.087E+02	3.99	B442	0 0 0 0 0	
2.183E+00	3.060E+02	5.99	B442	0 0 0 0 0	
2.149E+00	3.012E+02	9.99	B442	0 0 0 0 0	
2.254E+00	3.161E+02	10.99	B442	0 0 0 0 0	
2.250E+00	3.154E+02	11.99	B442	0 0 0 0 0	
3.200E+00	4.486E+02	12	F300	1 0 0 0 2	
2.234E+00	3.131E+02	14.99	B442	0 0 0 0 0	
2.191E+00	3.072E+02	19.99	B442	0 0 0 0 0	
2.156E+00	3.023E+02	24.99	B442	0 0 0 0 0	
2.193E+00	3.074E+02	29.99	B442	0 0 0 0 0	
2.218E+00	3.110E+02	34.99	B442	0 0 0 0 0	
2.233E+00	3.131E+02	39.99	B442	0 0 0 0 0	

876. $C_6H_{12}N_4O_2$
2,6-Dimethyldinitrosopiperazine
DMDNP
RN: 55380-34-2 **MP** (°C)**:**
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.066E+01	24	M031	1 1 1 1 1	

877. $C_6H_{12}N_5O_2PS_2$
Menazon
O,*O*-Dimethyl *S*-(4,6-diamino-1,3,5-triazinyl-2-methyl) dithiophosphate
RN: 78-57-9 **MP** (°C)**:**
MW: 281.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.532E-04	2.400E-01	20	M161	1 0 0 0 1	
3.551E-03	9.990E-01	ns	M061	0 0 0 0 0	

878. $C_6H_{12}O$
Pinacolone
3,3-Dimethyl-2-butanone
3,3-Dimethylbutanone-2
RN: 75-97-8 **MP** (°C)**:** –52.5
MW: 100.16 **BP** (°C)**:** 106.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.376E-01	2.380E+01	15	F300	1 0 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	
1.862E-01	1.865E+01	25	G030	1 2 0 0 2	
1.817E-01	1.820E+01	25	K072	1 0 1 1 1	
1.736E-01	1.739E+01	30	G030	1 2 0 0 2	

879. $C_6H_{12}O$
Cyclohexanol
1-Cyclohexanol
Naxol
Cyclohexyl alcoho
Adrona
Hydrophenol
RN: 108-93-0 **MP** (°C)**:** 23
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.357E-01	5.366E+01	11	F052	1 1 1 0 2	
5.391E-01	5.400E+01	11	F300	1 0 0 0 1	
1.296E-02	1.298E+00	20	D052	1 1 0 0 1	*sic*
3.283E-01	3.288E+01	25	B019	1 0 1 2 0	
3.283E-01	3.288E+01	25	B092	2 1 1 1 2	
3.469E-01	3.475E+01	25	C108	2 2 2 2 2	
3.800E-01	3.806E+01	25	F044	1 0 0 0 1	
3.766E-01	3.772E+01	25	H028	2 0 2 0 2	
3.655E-01	3.661E+01	35	C108	2 2 2 2 2	
3.264E-01	3.269E+01	60	B092	2 1 1 1 2	
3.766E-01	3.772E+01	ns	A406	0 0 0 0 1	

880. $C_6H_{12}O$
Isopropylacetone
4-Methyl-2-pentanone
Methyl isobutyl ketone
RN: 108-10-1 **MP** (°C)**:** –80
MW: 100.16 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.070E-01	3.075E+01	0	G032	1 2 1 1 2	
2.310E-01	2.314E+01	10	G032	1 2 1 1 2	
1.871E-01	1.874E+01	20	D052	1 1 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	

(*continued*)

880. $C_6H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-01	1.961E+01	22.00	O005	2 0 2 2 0	
1.862E-01	1.865E+01	24.6	H121	2 0 0 0 1	
1.862E-01	1.865E+01	25	B060	2 0 1 1 1	
1.717E-01	1.720E+01	25	C329	1 1 1 1 1	average
1.871E-01	1.874E+01	25	G030	1 2 0 0 2	
2.340E-01	2.344E+01	25	K103	1 2 2 2 1	
1.862E-01	1.865E+01	25	L082	1 1 2 1 1	
1.736E-01	1.739E+01	25	L319	1 0 2 1 2	
1.817E-01	1.820E+01	25	M087	1 1 2 1 2	
1.669E-01	1.672E+01	25	R320	1 0 1 1 1	
1.746E-01	1.749E+01	30	G030	1 2 0 0 2	
1.660E-01	1.663E+01	30	G032	1 2 1 1 2	
1.410E-01	1.412E+01	50	G032	1 2 1 1 2	
4.720E+01	4.728E+03	53.0	R308	2 2 1 1 2	
1.669E-01	1.672E+01	70	L082	1 1 2 1 1	
1.370E-01	1.372E+01	75	G032	1 2 1 1 2	
4.300E+01	4.307E+03	97.0	R308	2 2 1 1 2	
4.088E+01	4.094E+03	108.0	R308	2 2 1 1 2	
3.902E+01	3.909E+03	120.0	R308	2 2 1 1 2	
3.333E-01	3.339E+01	125.0	R308	2 2 1 1 1	
5.278E-01	5.286E+01	151.0	R308	2 2 1 1 1	
3.425E+01	3.431E+03	153.0	R308	2 2 1 2 2	

881. $C_6H_{12}O$

2-Ethylbutanal
Ethyl butyraldehyde
2-Ethylbutyraldehyde
Diethyl acetaldehyde; ethyl butyraldehyde
Diethyl acetaldehyde
Ethyl butyraldehyde

RN: 97-96-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	3.025E+00	ns	S460	0 0 0 0 0	

882. $C_6H_{12}O$

Caproic aldehyde
Hexaldehyde
n-Hexanal

RN: 66-25-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-01	5.590E+01	0	C423	0 0 0 0 0	
4.493E-01	4.500E+01	4	C423	0 0 0 0 0	

(*continued*)

882. $C_6H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.155E-01	3.160E+01	10	C423	0 0 0 0 0	
4.992E-02	5.000E+00	25	A049	1 0 1 0 1	
1.907E-01	1.910E+01	25	C435	0 0 0 0 0	
4.792E-02	4.800E+00	25	J418	0 0 0 0 0	

883. $C_6H_{12}O$

4-Methyl-3-pentanone
4-Methylpentanone-3
RN: 565-69-5 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.601E-01	1.604E+01	20	G030	1 2 0 0 2	
1.495E-01	1.497E+01	25	G030	1 2 0 0 2	
1.398E-01	1.400E+01	30	G030	1 2 0 0 2	
1.549E-01	1.551E+01	ns	S460	0 0 0 0 0	

884. $C_6H_{12}O$

3-Methyl-2-pentanone
3-Methylpentanone-2
RN: 565-61-7 **MP** (°C)**:** <25
MW: 100.16 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-01	2.210E+01	20	G030	1 2 0 0 2	
2.044E-01	2.047E+01	25	G030	1 2 0 0 2	
1.890E-01	1.893E+01	30	G030	1 2 0 0 2	

885. $C_6H_{12}O$

3-Hexanone
Hexanone-3
RN: 589-38-8 **MP** (°C)**:** –55.5
MW: 100.16 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-01	1.546E+01	20	G030	1 2 0 0 2	
1.446E-01	1.449E+01	25	G030	1 2 0 0 2	
1.359E-01	1.361E+01	30	G030	1 2 0 0 2	

886. $C_6H_{12}O$
2-Methyl-4-penten-3-ol
2-Methylpenten-4-ol-3
RN: 4798-45-2 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-01	3.185E+01	20	G031	1 0 0 0 2	
2.964E-01	2.969E+01	25	G031	1 0 0 0 2	
2.804E-01	2.809E+01	30	G031	1 0 0 0 2	

887. $C_6H_{12}O$
1-Hexen-3-ol
Hexen-1-ol-3
RN: 4798-44-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E-01	2.648E+01	20	G031	1 0 0 0 2	
2.454E-01	2.458E+01	25	G031	1 0 0 0 2	
2.302E-01	2.306E+01	30	G031	1 0 0 0 2	

888. $C_6H_{12}O$
Methyl butyl ketone
2-Hexanone
Methyl *n*-butyl ketone
RN: 591-78-6 **MP** (°C)**:** –57
MW: 100.16 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-01	4.330E+01	0	C423	0 0 0 0 0	
3.335E-01	3.340E+01	4	C423	0 0 0 0 0	
2.386E-01	2.390E+01	10	C423	0 0 0 0 0	
2.040E-01	2.043E+01	10	G032	1 2 1 1 2	
2.192E-02	2.195E+00	20	D052	1 1 0 0 1	*sic*
1.717E-01	1.720E+01	20	G030	1 2 0 0 2	
1.617E-01	1.620E+01	25	C435	0 0 0 0 0	
1.611E-01	1.614E+01	25	G030	1 2 0 0 2	
1.997E-01	2.000E+01	25	J418	0 0 0 0 0	
3.320E-01	3.326E+01	25	P055	1 0 0 0 2	
1.505E-01	1.507E+01	30	G030	1 2 0 0 2	
1.450E-01	1.452E+01	30	G032	1 2 1 1 2	
1.475E-01	1.478E+01	38	J020	2 1 2 1 1	
1.240E-01	1.242E+01	50	G032	1 2 1 1 2	

889. $C_6H_{12}O$
4-Hexen-3-ol
Hexen-4-ol-3
RN: 4798-58-7 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-01	3.902E+01	20	G031	1 0 0 0 2	
3.664E-01	3.670E+01	25	G031	1 0 0 0 2	
3.451E-01	3.456E+01	30	G031	1 0 0 0 2	

890. $C_6H_{12}O_2$
3-Hydroxy-2,2-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2,2-dimethyl-
2,2-Dimethyltetrahydrofuran-3-ol
RN: 101398-19-0 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.826E-01	9.091E+01	rt	B066	0 2 0 0 1	

891. $C_6H_{12}O_2$
Diethylacetic acid
2-Ethylbutyric acid
2-Ethyl-butanoic acid
Ethylbutyric acid
RN: 88-09-5 **MP** (°C)**:** –15
MW: 116.16 **BP** (°C)**:** 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.147E-02	2.494E+00	25	O011	1 0 1 1 1	

892. $C_6H_{12}O_2$
n-Caproic acid
n-Capronsaeure
RN: 142-62-1 **MP** (°C)**:** –3.4
MW: 116.16 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.438E-02	8.640E+00	0	B136	1 0 2 1 2	
7.610E-02	8.840E+00	15	F300	1 0 0 0 2	
8.333E-02	9.680E+00	20	B136	1 0 2 1 2	
8.270E-02	9.607E+00	20	D041	1 0 0 0 1	
8.253E-02	9.587E+00	20	R001	1 1 1 1 2	
8.675E-02	1.008E+01	25	H028	2 0 2 0 2	

(*continued*)

892. $C_6H_{12}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.760E-02	1.018E+01	25	H122	1 0 0 0 2	
8.608E-02	9.999E+00	25	H339	2 2 1 2 2	
9.367E-02	1.088E+01	25	O011	1 0 1 1 1	
8.772E-02	1.019E+01	30	B136	1 0 2 1 2	
8.684E-02	1.009E+01	30	R001	1 1 1 1 2	
9.282E-02	1.078E+01	35	H339	2 2 1 2 2	
9.427E-02	1.095E+01	45	B136	1 0 2 1 2	
9.324E-02	1.083E+01	45	R001	1 1 1 1 2	
1.008E-01	1.171E+01	60	B136	1 0 2 1 2	
9.956E-02	1.156E+01	60	D041	1 0 0 0 2	
9.964E-02	1.157E+01	60	R001	1 1 1 1 2	
7.374E-02	8.566E+00	.0	R001	1 1 1 1 2	
8.692E-02	1.010E+01	ns	A406	0 0 0 0 1	

893. $C_6H_{12}O_2$

n-Butyl acetate
Essigsaeure-n-butyl ester
n-Butylacetat
Butyl acetate
1-Butyl acetate

RN: 123-86-4 **MP** (°C)**:** –90
MW: 116.16 **BP** (°C)**:** 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-02	4.282E+00	20	D052	1 1 0 0 0	
8.609E-02	1.000E+01	22	F300	1 0 0 0 0	
5.814E-02	6.754E+00	25	B060	2 0 1 1 1	
7.171E-02	8.330E+00	25	L319	1 0 2 1 2	
1.935E-01	2.248E+01	25	P055	1 0 0 0 1	
2.489E-02	2.892E+00	30	N330	2 2 2 1 2	
7.679E-02	8.920E+00	30	R318	1 1 0 1 0	
5.020E-02	5.831E+00	37	E028	1 0 1 1 2	
5.899E-02	6.853E+00	50	O012	1 2 1 1 2	

894. $C_6H_{12}O_2$

Pentyl formate
n-Amyl formate

RN: 638-49-3 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	2.904E+00	22	S006	1 0 0 0 1	

895. $C_6H_{12}O_2$
Ethyl butyrate
Butanoic acid ethyl ester
Ethyl butanoate
Butyric ether
RN: 105-54-4 **MP** (°C)**:** –135.4
MW: 116.16 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-02	2.800E+00	0	C423	0 0 0 0 0	
2.763E-02	3.210E+00	4	C423	0 0 0 0 0	
3.151E-02	3.660E+00	10	C423	0 0 0 0 0	
4.198E-02	4.876E+00	20	D052	1 1 0 0 1	
5.310E-02	6.168E+00	22	F001	1 0 1 2 2	
4.300E-02	4.995E+00	22	S006	1 0 0 0 1	
3.702E-02	4.300E+00	25	C435	0 0 0 0 0	
6.832E-02	7.937E+00	30	R318	1 1 0 1 0	

896. $C_6H_{12}O_2$
sec-Butyl acetate
DL-*sec*-Butyl acetate
RN: 105-46-4 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.305E-02	6.162E+00	20	D052	1 1 0 0 0	

897. $C_6H_{12}O_2$
3-Hydroxy-2,5-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2,5-dimethyl-
RN: 30003-26-0 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.435E+00	1.667E+02	rt	B066	0 2 0 0 1	

898. $C_6H_{12}O_2$
Propyl propionate
Propionic acid *N*-propyl ester
n-Propyl propionate
RN: 106-36-5 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.808E+00	22	S006	1 0 0 0 0	

899. $C_6H_{12}O_2$
Isobutyl acetate
Acetic acid isobutyl ester
Essigsaeureisobutyl ester
RN: 110-19-0 **MP** (°C)**:** –99
MW: 116.16 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.502E-02	7.553E+00	14.60	L310	2 2 1 1 2	
5.729E-02	6.655E+00	20	D052	1 1 0 0 1	
5.800E-02	6.737E+00	20	F001	1 0 1 2 1	
5.768E-02	6.700E+00	20	F300	1 0 0 0 1	
6.154E-02	7.149E+00	24.90	L310	2 2 1 1 2	
5.390E-02	6.261E+00	25	B060	2 0 1 1 1	
5.967E-02	6.932E+00	47.90	L310	2 2 1 1 2	
6.154E-02	7.149E+00	67.60	L310	2 2 1 1 2	
6.493E-02	7.543E+00	74.90	L310	2 2 1 1 2	
6.502E-02	7.553E+00	75.20	L310	2 2 1 1 2	
6.875E-02	7.986E+00	84.80	L310	2 2 1 1 2	
7.205E-02	8.369E+00	93.20	L310	2 2 1 1 2	
8.253E-02	9.587E+00	111.50	L310	2 2 1 1 2	
8.540E-02	9.921E+00	115.70	L310	2 2 1 1 2	
1.026E-01	1.192E+01	147.10	L310	2 2 1 1 2	

900. $C_6H_{12}O_3$
Paraldehyde
Paraldehyd
RN: 123-63-7 **MP** (°C)**:** 12.6
MW: 132.16 **BP** (°C)**:** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.853E-01	1.170E+02	8.5	P059	1 1 1 0 1	
8.377E-01	1.107E+02	11.5	P059	1 1 1 0 1	
8.287E-01	1.095E+02	12.0	P059	1 1 1 0 1	
8.323E-01	1.100E+02	13	F300	1 0 0 0 1	
8.047E-01	1.063E+02	13.5	P059	1 1 1 0 1	
7.621E-01	1.007E+02	17.0	P059	1 1 1 0 1	
6.311E-01	8.341E+01	27.0	P059	1 1 1 0 1	
8.475E-01	1.120E+02	30	F300	1 0 0 0 2	
5.377E-01	7.106E+01	40.0	P059	1 1 1 0 1	
5.246E-01	6.933E+01	42.5	P059	1 1 1 0 1	
4.283E-01	5.660E+01	68.0	P059	1 1 1 0 1	
4.148E-01	5.482E+01	75.0	P059	1 1 1 0 1	
4.540E-01	6.000E+01	100	F300	1 0 0 0 0	

901. $C_6H_{12}O_3$
2-Ethoxyethyl acetate
Cellosolve acetate
RN: 111-15-9 **MP** (°C)**:** –61
MW: 132.16 **BP** (°C)**:** 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.499E+00	1.981E+02	20	D052	1 1 0 0 2	
1.415E+00	1.870E+02	20	M062	1 0 0 0 2	

902. $C_6H_{12}O_3$
Methyl β-ethoxypropionate
Methyl 3-ethoxypropionate
3-Ethoxypropionic acid methyl ester
RN: 14144-33-3 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.621E-01	1.007E+02	25	D002	1 2 1 1 2	
7.621E-01	1.007E+02	25	R034	0 0 0 0 2	

903. $C_6H_{12}O_5$
D-Quercitol
D-Quercit
RN: 488-73-3 **MP** (°C)**:** 234
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.701E-01	1.100E+02	20	F300	1 0 0 0 2	

904. $C_6H_{12}O_5$
Rhamnose
α-L-Rhamnose
6-Deoxy-L-mannose
L-Mannomethylose
L-Rhamnose
RN: 3615-41-6 **MP** (°C)**:** 82
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.212E+00	3.631E+02	18	D041	1 0 0 0 1	
3.177E+00	5.215E+02	40	D041	1 0 0 0 1	

905. $C_6H_{12}O_6$
D-Inositol
D(+)-Inositol
D-Chiro-inositol
(+)-Chiro-inositol
RN: 643-12-9 **MP** (°C)**:** 249.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	4.034E+02	11	F300	1 0 0 0 2	

906. $C_6H_{12}O_6$
D-Mannose
D-(+)-Mannose
Seminose
Carubinose
RN: 3458-28-4 **MP** (°C)**:** 132
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.956E+00	7.126E+02	17	D041	1 0 0 0 2	
3.957E+00	7.128E+02	17	F300	1 0 0 0 2	
2.399E+00	4.322E+02	25	G317	0 0 0 0 0	

907. $C_6H_{12}O_6$
Glucose
D-Glucose
D(+)-Glucose
Staleydex 111
Staleydex 333
RN: 50-99-7 **MP** (°C)**:** 146
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.954E+00	3.520E+02	.50	J019	1 0 1 2 2	
1.749E+00	3.151E+02	0	M043	1 0 0 0 1	
2.286E+00	4.118E+02	10	M043	1 0 0 0 1	
2.271E+00	4.091E+02	10.0	Y020	1 1 2 1 2	
3.365E+00	6.063E+02	15	D041	1 0 0 0 2	
2.660E+00	4.792E+02	20	M043	1 0 0 0 1	
2.314E+00	4.168E+02	20.0	Y020	1 1 2 1 2	
3.033E+00	5.464E+02	30	J019	1 0 1 2 2	
3.031E+00	5.460E+02	30	K122	1 1 1 1 2	
3.028E+00	5.455E+02	30	M043	1 0 0 0 2	
2.355E+00	4.244E+02	30.0	Y020	1 1 2 1 2	
1.901E+00	3.425E+02	30.50	M137	2 1 2 2 2	
2.042E+00	3.678E+02	35	B354	0 0 0 0 0	

(*continued*)

907. $C_6H_{12}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.416E+00	6.154E+02	40	M043	1 0 0 0 2	
2.396E+00	4.317E+02	40.0	Y020	1 1 2 1 2	
3.936E+00	7.091E+02	50	J019	1 0 1 2 2	
2.436E+00	4.388E+02	50.0	Y020	1 1 2 1 2	
4.090E+00	7.368E+02	60	M043	1 0 0 0 2	
4.005E+00	7.215E+02	70	A420	0 0 0 0 0	
4.523E+00	8.148E+02	80	M043	1 0 0 0 2	
2.227E+00	4.012E+02	.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	rt	D021	0 0 1 1 2	

908. $C_6H_{12}O_6$
Fructose
D-Fructose
D-(–)-Fructose
D-(–)-Levulose
Krystar 300
Nevulose
RN: 57-48-7 **MP** (°C)**:** 129
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	4.286E+02	0	M043	1 0 0 0 1	
4.318E+00	7.780E+02	20	F300	1 0 0 0 2	
2.467E+00	4.444E+02	20	M043	1 0 0 0 1	
4.524E+00	8.150E+02	30	K122	1 1 1 1 2	
4.524E+00	8.150E+02	30	K135	1 1 1 1 2	
2.448E+01	4.410E+03	30	K136	1 1 1 1 2	
2.550E+00	4.595E+02	40	M043	1 0 0 0 1	
2.629E+00	4.737E+02	60	M043	1 0 0 0 1	
4.709E+00	8.484E+02	70	A420	0 0 0 0 0	

909. $C_6H_{12}O_6$
Tagatose
Lyxo-2-hexulose
DL-Tagatose
RN: 17598-81-1 **MP** (°C)**:**
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.084E+00	3.755E+02	22	F300	1 0 0 0 2	

910. $C_6H_{12}O_6$
D-Galactose
Galactose
(+)-Galactose
D(+)-Galactose
RN: 59-23-4 **MP** (°C)**:** 169
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.046E-01	9.091E+01	0	D041	1 0 0 0 1	
2.247E+00	4.048E+02	25	D041	1 0 0 0 1	
2.253E+00	4.058E+02	rt	D021	0 0 1 1 2	

911. $C_6H_{12}O_6$
L-Sorbose
Sorbose
L-1,3,4,5,6-Pentahydroxyhexan-2-one
L-Xylo-2-hexulose
RN: 87-79-6 **MP** (°C)**:** 165
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.970E+00	3.548E+02	17	D041	1 0 0 0 1	
1.998E+00	3.600E+02	17	F300	1 0 0 0 1	

912. $C_6H_{12}O_6$
Inositol
Mesoinosit
cis-1,2,3,5-*trans*-4,6-Cyclohexanehexol
Dambose
Nucite
Phaseomannite
RN: 87-89-8 **MP** (°C)**:** 226
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.788E-01	1.403E+02	19	F300	1 0 0 0 2	
8.267E-01	1.489E+02	20	D041	1 0 0 0 2	
7.771E-01	1.400E+02	25	M054	1 0 0 0 1	
7.771E-01	1.400E+02	ns	L335	0 0 0 0 2	
7.762E-01	1.398E+02	ns	R424	0 0 0 0 0	

913. $C_6H_{12}O_6$
α-Glucose
α-D-Glucose
D-α-Glucose
Dextrose
RN: 492-62-6 **MP** (°C)**:** 154.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.355E+00	2.441E+02	0	D041	1 0 0 0 2	
2.019E+00	3.638E+02	10.0	Y020	1 1 2 1 2	
2.775E+00	5.000E+02	20	F300	1 0 0 0 0	
2.096E+00	3.775E+02	20.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	25	D041	1 0 0 0 2	
2.170E+00	3.909E+02	30.0	Y020	1 1 2 1 2	
2.242E+00	4.040E+02	40.0	Y020	1 1 2 1 2	
2.313E+00	4.168E+02	50.0	Y020	1 1 2 1 2	
2.346E+00	4.227E+02	54.7	Y020	1 1 2 1 2	
1.942E+00	3.498E+02	.0	Y020	1 1 2 1 2	

914. $C_6H_{12}O_6.H_2O$
Glucose (monohydrate)
RN: 50-99-7 **MP** (°C)**:** 83
MW: 198.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E+00	2.871E+02	10.0	Y020	1 1 2 1 2	
1.619E+00	3.209E+02	20.0	Y020	1 1 2 1 2	
1.781E+00	3.530E+02	30.0	Y020	1 1 2 1 2	
1.933E+00	3.831E+02	40.0	Y020	1 1 2 1 2	
2.072E+00	4.106E+02	50.0	Y020	1 1 2 1 2	
1.784E+00	3.536E+02	73.2	Y020	1 1 2 1 2	
1.274E+00	2.525E+02	.0	Y020	1 1 2 1 2	

915. $C_6H_{12}O_7$
Scyllitol
Scyllit
Quercinitol
Cocositol
RN: 488-59-5 **MP** (°C)**:** 253
MW: 196.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.149E-02	1.010E+01	18	F300	1 0 0 0 2	

916. $C_6H_{13}Br$

1-Bromohexane
Hexyl bromide

RN: 111-25-1 **MP** (°C)**:** –84.7
MW: 165.08 **BP** (°C)**:** 155.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-04	2.575E-02	25	M342	1 0 1 1 2	

917. $C_6H_{13}N$

1-Methylpiperidine
N-Methylpiperidine

RN: 626-67-5 **MP** (°C)**:** –18
MW: 99.18 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+1.70E+00	+1.68E+02	ns	S460	0 0 0 0 0	

918. $C_6H_{13}NO$

Caproamide
n-Capronsaeure-amid
Hexanamide
Hexanoic acid, amide

RN: 628-02-4 **MP** (°C)**:** 99
MW: 115.18 **BP** (°C)**:** 255

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-01	1.854E+01	6	H059	0 0 0 0 0	
2.030E-01	2.338E+01	16	H059	0 0 0 0 0	
2.580E-01	2.972E+01	25	H059	0 0 0 0 0	
2.750E-01	3.167E+01	29	H059	0 0 0 0 0	
3.150E-01	3.628E+01	33	H059	0 0 0 0 0	
3.250E-01	3.743E+01	35	H059	0 0 0 0 0	
3.390E-01	3.904E+01	37	H059	0 0 0 0 0	
3.890E-01	4.480E+01	41	H059	0 0 0 0 0	

919. $C_6H_{13}NO_2$

L-Norleucine
Norleucine
α-Aminocaproic acid

RN: 327-57-1 **MP** (°C)**:** 327dec
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-01	1.710E+01	23	K060	1 2 0 0 2	
1.127E-01	1.478E+01	25	D041	1 0 0 0 1	
8.700E-02	1.141E+01	25	E015	1 2 1 1 1	
1.232E-01	1.616E+01	25	K031	2 1 2 1 2	

920. $C_6H_{13}NO_2$
L-Leucine
L(–)-Leucine
Leucine
2-Amino-4-methylpentanoic acid
L-2-Amino-4-methylpentanoic acid
(2*S*)-α-Leucine
RN: 61-90-5 **MP** (°C)**:** 286–288
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.692E-01	2.220E+01	0	F300	1 0 0 0 2	
1.740E-01	2.282E+01	15	D349	2 1 1 2 2	
1.601E-01	2.100E+01	20	B032	1 2 2 1 2	
1.800E-01	2.361E+01	20	D349	2 1 1 2 2	
1.695E-01	2.224E+01	21	P045	1 0 2 1 2	
1.772E-01	2.324E+01	24.99	C404	2 1 2 2 1	
1.640E-01	2.151E+01	25	B032	1 2 2 1 2	
1.712E-01	2.246E+01	25	C018	0 0 0 0 0	
1.851E-01	2.428E+01	25	C018	0 0 0 0 0	
1.700E-04	2.230E-02	25	C405	2 1 2 2 2	intrinsic zwit
1.883E-01	2.470E+01	25	D016	1 0 0 0 2	
1.634E-01	2.143E+01	25	D041	1 0 0 0 2	
1.860E-01	2.440E+01	25	D349	2 1 1 2 2	
1.807E-01	2.370E+01	25	F300	1 0 0 0 2	
1.626E-01	2.133E+01	25	G092	2 1 1 1 1	
1.626E-01	2.133E+01	25	G315	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N024	0 0 0 0 0	
1.654E-01	2.170E+01	25.1	N025	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N026	0 0 0 0 0	
1.612E-01	2.114E+01	25.1	N027	1 1 2 2 2	
1.765E-01	2.315E+01	27	D036	0 0 0 0 0	
1.601E-01	2.100E+01	27	D036	0 0 0 0 0	
1.682E-01	2.206E+01	29.80	B032	1 2 2 1 2	
1.907E-01	2.502E+01	34.99	C404	2 1 2 2 1	
2.041E-01	2.677E+01	44.99	C404	2 1 2 2 1	
2.142E-01	2.810E+01	50	F300	1 0 0 0 2	
2.805E-01	3.679E+01	75	D041	1 0 0 0 2	
2.805E-01	3.680E+01	75	F300	1 0 0 0 2	
2.886E-01	3.786E+01	92	M160	2 1 1 1 0	
4.071E-01	5.340E+01	100	F300	1 0 0 0 2	
4.069E-01	5.337E+01	99.99	P349	0 0 0 0 0	
1.830E-01	2.400E+01	ns	D072	0 0 0 0 1	

921. $C_6H_{13}NO_2$
L-*allo*-Isoleucine
Alloisoleucine
RN: 1509-34-8 **MP** (°C)**:** >280
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-01	2.818E+01	20	D041	1 0 0 0 1	

922. $C_6H_{13}NO_2$
D-Leucine
D-2-Amino-4-methylvaleric acid
D-2-Amino-4-methylpentanoic acid
RN: 328-38-1 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-01	2.153E+01	25	D041	1 0 0 0 2	
1.975E-01	2.591E+01	50	D041	1 0 0 0 2	

923. $C_6H_{13}NO_2$
D-Norleucine
D-2-Amino-*n*-caproic acid
D-2-Aminohexanoic acid
RN: 327-56-0 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.201E-01	1.575E+01	19	D041	1 0 0 0 1	

924. $C_6H_{13}NO_2$
tert-Amyl carbamate
tert-Pentyl carbamate
RN: 590-60-3 **MP** (°C)**:** 85
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-01	2.099E+01	37	H006	1 2 2 1 1	

925. $C_6H_{13}NO_2$
n-Amyl carbamate
n-Pentyl carbamate
O-Pentyl carbamate
RN: 638-42-6 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.460E+00	37	H006	1 2 2 1 1	

926. $C_6H_{13}NO_2$
Isopentyl urethane
Isoamylurethan
Isoamylurethane
RN: 543-86-2 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.660E-02	4.801E+00	15.5	F001	1 0 1 2 2	

927. $C_6H_{13}NO_2$
ε-Aminocaproic acid
6-Aminocaproic acid
ε-Amino-capronsaeure
RN: 60-32-2 **MP** (°C)**:** 205
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.848E+00	5.048E+02	25	M024	1 2 0 1 2	

928. $C_6H_{13}NO_2$
DL-Norleucine
DL-2-Amino-*n*-caproic acid
2-Aminohexanoic acid
DL-2-Aminohexanoic acid
RN: 616-06-8 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-02	9.003E+00	0	D018	2 2 2 1 2	
8.660E-02	1.136E+01	25	C018	0 0 0 0 0	
8.767E-02	1.150E+01	25	D016	1 0 0 0 2	
8.906E-02	1.168E+01	25	D018	2 2 2 1 2	
8.891E-02	1.166E+01	25	D041	1 0 0 0 2	
8.118E-02	1.065E+01	25	K031	2 1 2 1 2	
8.660E-02	1.136E+01	25	M024	1 2 0 1 2	
1.348E-01	1.768E+01	50	D018	2 2 2 1 2	
2.135E-01	2.800E+01	75	D018	2 2 2 1 2	
2.134E-01	2.799E+01	75	D041	1 0 0 0 2	
3.788E-01	4.969E+01	99.99	P349	0 0 0 0 0	

929. $C_6H_{13}NO_2$
L-Isoleucine
L(+)-Isoleucin
Isoleucine
RN: 73-32-5 **MP** (°C)**:** 288
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.844E-01	3.730E+01	15.50	F300	1 0 0 0 2	
2.533E-01	3.323E+01	20	B032	1 2 2 1 2	
2.619E-01	3.435E+01	25	B032	1 2 2 1 2	
3.017E-01	3.957E+01	25	D041	1 0 0 0 2	
2.458E-01	3.224E+01	25	G433	0 0 0 0 0	
2.364E-01	3.101E+01	25	O316	1 0 1 2 2	
2.358E-01	3.093E+01	25	O316	1 0 1 2 2	
2.714E-01	3.560E+01	27	D036	0 0 0 0 0	
2.690E-01	3.528E+01	29.80	B032	1 2 2 1 2	
4.369E-01	5.732E+01	75	D041	1 0 0 0 2	
3.801E-01	4.985E+01	84	M160	2 1 1 1 0	

930. $C_6H_{13}NO_2$
α-Hydroxycaproamide
Hexanamide, 2-hydroxy-
2-Hydroxyhexanamide
RN: 66461-73-2 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.300E-02	1.089E+01	25	M008	1 0 0 0 2	

931. $C_6H_{13}NO_2$
N-Propylurethane
Propylurethan
n-Propyl urethane
RN: 623-85-8 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.475E-01	9.805E+01	15.5	F001	1 0 1 2 2	

932. $C_6H_{13}NO_2$

DL-Isoleucine
DL-2-Amino-3-methylpentanoic acid
RN: 443-79-8 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-01	1.720E+01	0	D018	2 2 2 1 2	
1.632E-01	2.141E+01	25	D018	2 2 2 1 2	
1.662E-01	2.180E+01	25	D041	1 0 0 0 2	
2.235E-01	2.931E+01	50	D018	2 2 2 1 2	
3.510E-01	4.605E+01	75	D018	2 2 2 1 2	
3.357E-01	4.404E+01	75	D041	1 0 0 0 2	
5.517E-01	7.237E+01	99.99	P349	0 0 0 0 0	

933. $C_6H_{13}NO_2$

DL-Leucine
DL-2-Amino-4-methylvaleric acid
DL-2-Amino-4-methylpentanoic acid
RN: 328-39-2 **MP** (°C)**:** 295
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-02	8.735E+00	0	D018	2 2 2 1 2	
6.022E-02	7.900E+00	0	F300	1 0 0 0 1	
7.433E-02	9.750E+00	25	C018	0 0 0 0 0	
7.517E-02	9.860E+00	25	D016	1 0 0 0 2	
8.898E-02	1.167E+01	25	D018	2 2 2 1 2	
7.481E-02	9.813E+00	25	D041	1 0 0 0 2	
7.471E-02	9.800E+00	25	F300	1 0 0 0 1	
1.321E-01	1.733E+01	50	D018	2 2 2 1 2	
1.060E-01	1.390E+01	50	F300	1 0 0 0 2	
2.105E-01	2.762E+01	75	D018	2 2 2 1 2	
1.696E-01	2.225E+01	75	D041	1 0 0 0 2	
1.700E-01	2.230E+01	75	F300	1 0 0 0 2	
3.080E-01	4.040E+01	100	F300	1 0 0 0 2	
3.077E-01	4.036E+01	99.99	P349	0 0 0 0 0	
7.324E-02	9.607E+00	rt	H431	0 0 0 0 0	average

934. C_6H_{14}

Hexane
Normal hexane
n-Hexane
Skellysolve B
RN: 110-54-3 **MP** (°C)**:** –95
MW: 86.18 **BP** (°C)**:** 65

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-04	1.650E-02	0	P003	2 2 2 2 2	
1.900E-04	1.637E-02	4.0	N004	1 1 2 2 2	

(*continued*)

934. C_6H_{14} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-04	1.518E-02	14.0	N004	1 1 2 2 2	
1.600E-03	1.379E-01	15.5	F001	1 0 1 0 2	
6.382E-04	5.500E-02	16	D047	1 0 0 1 1	
1.427E-04	1.230E-02	25	A058	1 1 1 1 2	
1.624E-03	1.400E-01	25	A094	1 0 0 0 1	
1.625E-03	1.400E-01	25	K072	1 0 1 1 1	
1.857E-03	1.600E-01	25	K112	1 0 2 1 1	
1.860E-03	1.603E-01	25	K112	1 0 2 2 2	
1.099E-04	9.470E-03	25	K119	1 0 0 0 2	
1.427E-04	1.230E-02	25	L002	2 2 2 2 2	
1.102E-04	9.500E-03	25	M001	2 1 2 2 2	
1.102E-04	9.500E-03	25	M002	2 1 2 2 2	
1.102E-04	9.500E-03	25	M040	1 0 0 1 1	
1.625E-03v	1.400E-01	25	M087	1 1 2 1 1	
1.430E-04	1.232E-02	25	M342	1 0 1 1 2	
1.439E-04	1.240E-02	25	P003	2 2 2 2 2	
1.624E-03	1.400E-01	25	S012	2 0 2 2 1	
2.128E-04	1.834E-02	25.0	N004	1 1 2 2 2	
1.099E-04	9.470E-03	25.0	P051	2 1 1 2 2	
1.099E-04	9.470E-03	25.00	P007	2 1 2 2 2	
1.494E-04	1.288E-02	35.0	N004	1 1 2 2 2	
4.623E-02	3.984E+00	38	J020	2 0 2 1 0	*sic*
1.172E-04	1.010E-02	40.1	P051	2 1 1 2 2	
1.172E-04	1.010E-02	40.10	P007	2 1 2 2 2	
2.578E-04	2.221E-02	45.0	N004	1 1 2 2 2	
2.553E-03	2.200E-01	50	L097	1 1 1 1 1	
2.456E-04	2.116E-02	55.0	N004	1 1 2 2 2	
1.532E-04	1.320E-02	55.7	P051	2 1 1 2 2	
1.532E-04	1.320E-02	55.70	P007	2 1 2 2 2	
1.775E-04	1.530E-02	69.7	P051	2 1 1 2 2	average of 2
1.764E-04	1.520E-02	69.70	P007	2 1 2 2 2	
1.787E-04	1.540E-02	69.70	P007	2 1 2 2 2	
2.599E-04	2.240E-02	99.1	P051	2 1 1 2 2	
2.599E-04	2.240E-02	99.10	P007	2 1 2 2 2	
3.388E-04	2.920E-02	114.4	P051	2 1 1 2 2	
3.388E-04	2.920E-02	114.40	P007	2 1 2 2 2	
4.363E-04	3.760E-02	121.3	P051	2 1 1 2 2	
4.363E-04	3.760E-02	121.30	P007	2 1 2 2 2	
6.603E-04	5.690E-02	137.3	P051	2 1 1 2 2	
6.603E-04	5.690E-02	137.30	P007	2 1 2 2 2	
1.230E-03	1.060E-01	151.8	P051	2 1 1 2 2	
1.230E-03	1.060E-01	151.80	P007	2 1 2 2 2	
1.102E-04	9.500E-03	ns	H123	0 0 0 0 0	
1.392E-03	1.200E-01	ns	M010	0 0 0 0 1	
1.880E-04	1.620E-02	ns	M175	0 0 2 1 2	

935. C_6H_{14}

2,2-Dimethylbutane
Neohexane

RN: 75-83-2 **MP** (°C)**:** –100
MW: 86.18 **BP** (°C)**:** 50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.572E-04	3.940E-02	0	P003	2 2 2 2 2	
4.278E-04	3.686E-02	2.34	S461	0 0 0 0 0	
3.444E-04	2.968E-02	9.99	S461	0 0 0 0 0	
2.722E-04	2.346E-02	24.99	S461	0 0 0 0 0	
2.460E-04	2.120E-02	25	K119	1 0 0 0 2	
2.135E-04	1.840E-02	25	M001	2 1 2 2 2	
2.135E-04	1.840E-02	25	M002	2 1 2 2 2	
2.762E-04	2.380E-02	25	P003	2 2 2 2 2	
2.460E-04	2.120E-02	25	P051	2 1 1 2 2	
2.460E-04	2.120E-02	25.00	P007	2 1 2 2 2	
6.600E-04	5.687E-02	ns	J300	0 0 0 0 0	

936. C_6H_{14}

2,3-Dimethylbutane
Diisopropyl
1,1,2,2-Tetramethylethane

RN: 79-29-8 **MP** (°C)**:** –129
MW: 86.18 **BP** (°C)**:** 58

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.818E-04	3.290E-02	0	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25	K119	1 0 0 0 2	
2.611E-04	2.250E-02	25	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25.0	P051	2 1 1 2 2	
2.216E-04	1.910E-02	25.00	P007	2 1 2 2 2	
2.228E-04	1.920E-02	40.1	P051	2 1 1 2 2	
2.228E-04	1.920E-02	40.10	P007	2 1 2 2 2	
2.750E-04	2.370E-02	55.1	P051	2 1 1 2 2	
2.750E-04	2.370E-02	55.10	P007	2 1 2 2 2	
4.653E-04	4.010E-02	99.1	P051	2 1 1 2 2	
4.653E-04	4.010E-02	99.10	P007	2 1 2 2 2	
6.591E-04	5.680E-02	121.3	P051	2 1 1 2 2	
6.591E-04	5.680E-02	121.30	P007	2 1 2 2 2	
1.136E-03	9.790E-02	137.3	P051	2 1 1 2 2	
1.136E-03	9.790E-02	137.30	P007	2 1 2 2 2	
1.984E-03	1.710E-01	149.5	P051	2 1 1 2 2	
1.984E-03	1.710E-01	149.50	P007	2 1 2 2 2	

937. C_6H_{14}
2-Methylpentane
2-Metylopentan
RN: 107-83-5 **MP** (°C)**:** –154
MW: 86.18 **BP** (°C)**:** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.257E-04	1.945E-02	0	P003	2 2 2 2 2	
5.976E-04	5.150E-02	23	C332	0 0 0 0 0	
1.508E-04	1.300E-02	25	K119	1 0 0 0 2	
1.648E-04	1.420E-02	25	L002	2 2 2 2 2	
1.601E-04	1.380E-02	25	M001	2 1 2 2 2	
1.601E-04	1.380E-02	25	M002	2 1 2 2 2	
1.822E-04	1.570E-02	25	P003	2 2 2 2 2	
1.508E-04	1.300E-02	25.0	P051	2 1 1 2 2	
1.508E-04	1.300E-02	25.00	P007	2 1 2 2 2	
1.601E-04	1.380E-02	40.1	P051	2 1 1 2 2	
1.601E-04	1.380E-02	40.10	P007	2 1 2 2 2	
1.822E-04	1.570E-02	55.7	P051	2 1 1 2 2	
1.822E-04	1.570E-02	55.70	P007	2 1 2 2 2	
3.145E-04	2.710E-02	99.1	P051	2 1 1 2 2	
3.145E-04	2.710E-02	99.10	P007	2 1 2 2 2	
5.210E-04	4.490E-02	118.0	P051	2 1 1 2 2	
5.210E-04	4.490E-02	118.00	P007	2 1 2 2 2	
1.007E-03	8.680E-02	137.3	P051	2 1 1 2 2	
1.007E-03	8.680E-02	137.30	P007	2 1 2 2 2	
1.311E-03	1.130E-01	149.50	P007	2 1 2 2 2	

938. C_6H_{14}
3-Methylpentane
3-Metylopentan
RN: 96-14-0 **MP** (°C)**:** –118
MW: 86.18 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-04	2.150E-02	0	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	K119	1 0 0 0 2	
1.485E-04	1.280E-02	25	M001	2 1 2 2 2	
2.077E-04	1.790E-02	25	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	P051	2 1 1 2 2	
1.520E-04	1.310E-02	25.00	P007	2 1 2 2 2	
1.485E-04	1.280E-02	ns	H123	0 0 0 0 0	

939. $C_6H_{14}FO_3P$
Isofluorphate
Diisopropylfluorophosphate
Phosphorofluoridic acid bis(1-methylethyl) ester
Difluorophate
PF-3
T-1703
RN: 55-91-4 **MP** (°C)**:** –82
MW: 184.15 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.236E-02	1.517E+01	25	D041	1 0 0 0 2	

940. $C_6H_{14}NO_3PS_2$
Ethoate-methyl
O,*O*-Dimethyl *S*-(*N*-ethylcarbamoylmethyl) dithiophosphate
Fitios
RN: 116-01-8 **MP** (°C)**:** 66.1
MW: 243.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-02	8.500E+00	25	M061	1 0 0 0 1	
3.494E-02	8.500E+00	25	M161	1 0 0 0 1	

941. $C_6H_{14}N_2$
trans-2,5-Dimethylpiperazine
trans-2,5-Dimethyl-piperazin
RN: 2815-34-1 **MP** (°C)**:**
MW: 114.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.065E+00	3.500E+02	20	F300	1 0 0 0 1	

942. $C_6H_{14}N_2O$
Methyl-*n*-amylnitrosamine
N-Nitroso(methyl)pentylamine
RN: 13256-07-0 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-02	1.094E+01	24	D083	2 0 0 0 1	

943. $C_6H_{14}N_2O$
Di-*n*-propylnitrosamine
N-Nitroso-*N*-propyl-1-propanamine
Dipropylnitrosamine
NDPA
DPNA
Nitrosodipropylamine
RN: 621-64-7 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	9.895E+00	24	D083	2 0 0 0 1	

944. $C_6H_{14}N_2O$
Ethyl-*n*-butylnitrosamine
Nitroso-*N*-ethyl-*n*-butylamine
N-Nitroso-*N*-butylethylamine
N-Nitroso(ethyl)-*n*-butylamine
NEBA
Butanamine, *N*-ethyl-*N*-nitroso-
RN: 4549-44-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-02	1.198E+01	24	D083	2 0 0 0 1	

945. $C_6H_{14}N_2O$
Di-isopropylnitrosamine
2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso-
N-Nitrosodiisopropylamine
NdiPA
RN: 601-77-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.302E+01	24	D083	2 0 0 0 1	

946. $C_6H_{14}N_2O_2$
L(+)-Lysine
L(+)-Lysin
Lysine
RN: 56-87-1 **MP** (°C)**:** 224
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.995E+00	5.840E+02	27	D036	0 0 0 0 0	

947. $C_6H_{14}N_4O_2$
DL-Arginine
(±)-Arginine
RN: 7200-25-1 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.382E+00	2.407E+02	20	J303	0 0 0 0 0	
1.978E+00	3.445E+02	40	J303	0 0 0 0 0	
2.781E+00	4.844E+02	50	J303	0 0 0 0 0	
3.851E+00	6.709E+02	60	J303	0 0 0 0 0	

948. $C_6H_{14}N_4O_2$
L-Arginine
L(+)-Arginin
Arginine
RN: 74-79-3 **MP** (°C)**:** 244
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.559E-01	1.143E+02	10	H062	1 2 2 0 0	EFG
8.588E-01	1.496E+02	20	B032	1 2 2 1 2	
7.487E-01	1.304E+02	21	D041	1 0 0 0 1	
8.037E-01	1.400E+02	21	F300	1 0 0 0 0	average
1.044E+00	1.818E+02	25	B032	1 2 2 1 2	
9.230E-01	1.608E+02	25	G315	0 0 0 0 0	
3.060E+00	5.330E+02	27	D036	0 0 0 0 0	
1.241E+00	2.162E+02	29.80	B032	1 2 2 1 2	
1.111E+00	1.935E+02	30	H062	1 2 2 0 0	EFG
1.771E+00	3.084E+02	50	H062	1 2 2 0 0	EFG

949. $C_6H_{14}O$
3-Methyl-3-pentanol
Diethylmethylcarbinol
RN: 77-74-7 **MP** (°C)**:** –24
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-01	4.379E+01	9.8	S307	1 1 0 2 2	
3.346E-01	3.419E+01	19.5	S307	1 1 0 2 2	
4.500E-01	4.598E+01	20	G005	1 2 1 1 2	
3.999E-01	4.086E+01	25	G005	1 2 1 1 2	
3.264E-01	3.335E+01	29.8	S307	1 1 0 2 2	
3.592E-01	3.670E+01	30	G005	1 2 1 1 2	
2.647E-01	2.705E+01	39.8	S307	1 1 0 2 2	
2.331E-01	2.382E+01	49.7	S307	1 1 0 2 2	
1.938E-01	1.980E+01	59.5	S307	1 1 0 2 2	
1.834E-01	1.874E+01	70.1	S307	1 1 0 2 2	
1.787E-01	1.826E+01	80.1	S307	1 1 0 2 2	
1.617E-01	1.652E+01	90.4	S307	1 1 0 2 2	

950. $C_6H_{14}O$
Dipropyl ether
Propyl ether
Dipropylaether
Dipropylether
RN: 111-43-3 **MP** (°C)**:** –123
MW: 102.18 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.644E-02	5.767E+00	0	B002	2 1 1 2 2	
3.996E-02	4.083E+00	10	B002	2 1 1 2 2	
3.705E-02	3.786E+00	15	B002	2 1 1 2 2	
2.927E-02	2.991E+00	20	B002	2 1 1 2 2	
2.936E-02	3.000E+00	20	F300	1 0 0 0 0	
6.700E-02	6.846E+00	20	S006	1 0 0 0 1	
2.441E-02	2.494E+00	25	B002	2 1 1 2 2	
1.070E-01	1.093E+01	37	E028	1 0 1 1 2	

951. $C_6H_{14}O$
tert-Amyl methyl ether
Methyl *tert*-amyl ether
RN: 994-05-8 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-01	1.235E+01	20	E019	1 0 1 1 2	

952. $C_6H_{14}O$
Propyl isopropyl ether
Propyl-isopropyl-aether
RN: 627-08-7 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.285E-02	7.444E+00	10	B002	2 1 1 2 2	
7.242E-02	7.400E+00	10	F300	1 0 0 0 1	
5.837E-02	5.964E+00	15	B002	2 1 1 2 2	
5.872E-02	6.000E+00	15	F300	1 0 0 0 1	
4.966E-02	5.074E+00	20	B002	2 1 1 2 2	
4.578E-02	4.678E+00	25	B002	2 1 1 2 2	
4.600E-02	4.700E+00	25	F300	1 0 0 0 1	

953. $C_6H_{14}O$
Isohexyl alcohol
4-Methyl-1-pentanol
RN: 626-89-1 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-01	1.042E+01	20	H330	0 0 0 0 0	

954. $C_6H_{14}O$
4-Methyl-2-pentanol
i-Butylmethylcarbinol
Methyl amyl alcohol
RN: 108-11-2 **MP** (°C)**:** –90
MW: 102.18 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.684E-01	2.743E+01	0	S307	1 1 0 2 2	
2.004E-01	2.047E+01	9.7	S307	1 1 0 2 2	
1.664E-01	1.701E+01	20	D052	1 1 0 0 2	
1.721E-01	1.759E+01	20	G005	1 2 1 1 2	
1.570E-01	1.604E+01	20.0	S307	1 1 0 2 2	
1.636E-01	1.672E+01	25	C093	2 1 1 1 1	
1.579E-01	1.614E+01	25	G005	1 2 1 1 2	
1.465E-01	1.497E+01	30	G005	1 2 1 1 2	
1.475E-01	1.507E+01	30.0	S307	1 1 0 2 2	
1.246E-01	1.274E+01	40.3	S307	1 1 0 2 2	
1.151E-01	1.176E+01	50.0	S307	1 1 0 2 2	
1.074E-01	1.098E+01	60.1	S307	1 1 0 2 2	
1.094E-01	1.117E+01	70.2	S307	1 1 0 2 2	
1.199E-01	1.225E+01	80.2	S307	1 1 0 2 2	
1.132E-01	1.156E+01	90.2	S307	1 1 0 2 2	

955. $C_6H_{14}O$
2,2-Dimethyl-3-butanol
t-Butylmethylcarbinol
RN: 464-07-3 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.517E-01	2.572E+01	20	G005	1 2 1 1 2	
2.322E-01	2.372E+01	25	G005	1 2 1 1 2	
2.163E-01	2.210E+01	30	G005	1 2 1 1 2	

956. $C_6H_{14}O$
1-Hexanol
n-Hexanol
Amyl carbinol
Caproic alcohol
n-Hexyl alcohol
RN: 111-27-3 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.173E-01	2.220E+01	0	C423	0 0 0 0 0	
7.864E-02	8.035E+00	0	E029	1 2 0 1 1	
9.344E-02	9.548E+00	0	S307	1 1 0 2 2	
1.732E-01	1.770E+01	4	C423	0 0 0 0 0	
7.706E-02	7.873E+00	5.54	H110	2 2 2 2 2	
7.487E-02	7.650E+00	6.84	H110	2 2 2 2 2	
7.213E-02	7.370E+00	8.64	H110	2 2 2 2 2	
1.223E-01	1.250E+01	10	C423	0 0 0 0 0	
6.803E-02	6.951E+00	10	E029	1 2 0 1 1	
7.372E-02	7.533E+00	10.2	S307	1 1 0 2 2	
6.906E-02	7.057E+00	11.04	H110	2 2 2 2 2	
6.671E-02	6.816E+00	12.94	H110	2 2 2 2 2	
6.506E-02	6.648E+00	14.64	H110	2 2 2 2 2	
6.287E-02	6.424E+00	17.04	H110	2 2 2 2 2	
6.861E-02	7.011E+00	20	A015	1 2 1 1 2	
6.224E-02	6.359E+00	20	E029	1 2 0 1 1	
6.070E-02	6.202E+00	20	H330	0 0 0 0 0	
4.869E-02	4.975E+00	20	L049	1 1 2 1 0	
5.150E-02	5.262E+00	20	P073	1 0 0 1 2	
6.475E-02	6.616E+00	20.0	S307	1 1 0 2 2	
5.991E-02	6.121E+00	20.74	H110	2 2 2 2 2	
5.854E-02	5.981E+00	22.94	H110	2 2 2 2 2	
6.250E-02	6.386E+00	24	H345	0 0 0 0 0	
6.069E-02	6.201E+00	25	B038	1 2 1 1 2	
5.644E-02	5.767E+00	25	B060	2 0 1 1 1	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.047E-02	7.200E+00	25	C435	0 0 0 0 0	
1.000E+00	1.022E+02	25	F044	1 0 0 0 0	EFG
8.000E-02	8.174E+00	25	G075	1 0 1 0 0	
5.900E-02	6.028E+00	25	K025	2 2 1 1 2	
8.922E-02	9.116E+00	25	M323	2 2 1 1 2	
5.711E-02	5.835E+00	25.04	H110	2 2 2 2 2	
5.640E-02	5.762E+00	26.94	H110	2 2 2 2 2	
5.579E-02	5.701E+00	28.94	H110	2 2 2 2 2	
5.431E-02	5.549E+00	29.7	S307	1 1 0 2 2	
6.320E-02	6.458E+00	30	C091	1 2 1 1 1	
5.740E-02	5.865E+00	30	E029	1 2 0 1 1	
5.517E-02	5.637E+00	30.94	H110	2 2 2 2 2	
5.440E-02	5.558E+00	33.04	H110	2 2 2 2 2	
5.005E-02	5.114E+00	39.8	S307	1 1 0 2 2	
5.257E-02	5.371E+00	40	E029	1 2 0 1 1	

(*continued*)

956. $C_6H_{14}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.869E-02	4.975E+00	50	E029	1 2 0 1 1	
4.840E-02	4.945E+00	50.0	S307	1 1 0 2 2	
5.063E-02	5.173E+00	60	E029	1 2 0 1 1	
5.043E-02	5.153E+00	60.0	S307	1 1 0 2 2	
5.450E-02	5.569E+00	70	E029	1 2 0 1 1	
5.540E-02	5.661E+00	70	F001	1 0 1 0 2	
5.615E-02	5.737E+00	70.3	S307	1 1 0 2 2	
5.934E-02	6.063E+00	80	E029	1 2 0 1 1	
6.080E-02	6.212E+00	80	F001	1 0 1 0 2	
6.079E-02	6.211E+00	80.3	S307	1 1 0 2 2	
6.707E-02	6.853E+00	90	E029	1 2 0 1 1	
6.660E-02	6.805E+00	90	F001	1 0 1 0 2	
6.204E-02	6.340E+00	90.3	S307	1 1 0 2 2	
7.767E-02	7.937E+00	100	E029	1 2 0 1 1	
7.690E-02	7.857E+00	100	F001	1 0 1 0 2	
8.826E-02	9.018E+00	110	E029	1 2 0 1 1	
8.720E-02	8.910E+00	110	F001	1 0 1 0 2	
1.007E-01	1.029E+01	120	E029	1 2 0 1 2	
1.151E-01	1.176E+01	130	E029	1 2 0 1 2	
1.323E-01	1.351E+01	140	E029	1 2 0 1 2	
1.570E-01	1.604E+01	150	E029	1 2 0 1 2	
1.966E-01	2.009E+01	160	E029	1 2 0 1 2	
2.573E-01	2.629E+01	170	E029	1 2 0 1 2	
3.410E-01	3.484E+01	180	E029	1 2 0 1 2	
4.545E-01	4.644E+01	190	E029	1 2 0 1 2	
6.188E-01	6.323E+01	200	E029	1 2 0 1 2	
8.654E-01	8.842E+01	210	E029	1 2 0 1 2	
1.372E+00	1.402E+02	220	E029	1 2 0 1 2	
6.114E-02	6.247E+00	ns	L003	0 0 2 1 2	

957. $C_6H_{14}O$

2-Hexanol
n-Butylmethylcarbinol
1-Methyl pentanol

RN: 626-93-7 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.975E-01	2.018E+01	0	S307	1 1 0 2 2	
1.617E-01	1.652E+01	10.1	S307	1 1 0 2 2	
1.246E-01	1.274E+01	19.8	S307	1 1 0 2 2	
1.456E-01	1.488E+01	20	G005	1 2 1 1 2	
1.690E-01	1.727E+01	20	H330	0 0 0 0 0	
1.323E-01	1.351E+01	25	G005	1 2 1 1 2	
1.141E-01	1.166E+01	29.9	S307	1 1 0 2 2	
1.237E-01	1.264E+01	30	G005	1 2 1 1 2	
1.055E-01	1.078E+01	40.0	S307	1 1 0 2 2	
9.306E-02	9.509E+00	50.0	S307	1 1 0 2 2	

(*continued*)

957. $C_6H_{14}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.826E-02	9.018E+00	60.2	S307	1 1 0 2 2	
9.498E-02	9.705E+00	70.0	S307	1 1 0 2 2	
1.094E-01	1.117E+01	80.1	S307	1 1 0 2 2	
9.114E-02	9.312E+00	90.2	S307	1 1 0 2 2	

958. $C_6H_{14}O$

2,2-Dimethyl-1-butanol
t-Pentylcarbinol
RN: 1185-33-7 **MP** (°C)**:** –35
MW: 102.18 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.960E-02	8.133E+00	20	G005	1 2 1 1 1	
7.382E-02	7.543E+00	25	G005	1 2 1 1 1	
6.900E-02	7.050E+00	30	G005	1 2 1 1 1	

959. $C_6H_{14}O$

2,3-Dimethyl-1-butanol
Dimethyl-*i*-propylcarbinol
Dimethyl-isopropylcarbinol
RN: 594-60-5 **MP** (°C)**:** –14
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.349E-01	4.443E+01	20	G005	1 2 1 1 2	
3.927E-01	4.012E+01	25	G005	1 2 1 1 2	
3.547E-01	3.624E+01	30	G005	1 2 1 1 2	

960. $C_6H_{14}O$

Isopropyl ether
Diisopropyl ether
RN: 108-20-3 **MP** (°C)**:** –60
MW: 102.18 **BP** (°C)**:** 68.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E-01	1.381E+01	24.6	H121	2 0 0 0 1	
8.730E-02	8.920E+00	25	F048	2 0 0 0 0	
7.920E-02	8.092E+00	37	E028	1 0 1 1 2	

961. $C_6H_{14}O$
2-Ethyl-1-butanol
2-Ethylbutanol
RN: 97-95-0 **MP** (°C)**:** –15
MW: 102.18 **BP** (°C)**:** 146

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.127E-02	6.261E+00	20	D052	1 1 0 0 1	
3.899E-02	3.984E+00	25	C093	2 1 1 1 0	

962. $C_6H_{14}O$
3-Methyl-2-pentanol
3-Methyl-2-pentyl alcohol
RN: 565-60-6 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.004E-01	2.047E+01	20	G005	1 2 1 1 2	
1.863E-01	1.903E+01	25	G005	1 2 1 1 2	
1.721E-01	1.759E+01	30	G005	1 2 1 1 2	

963. $C_6H_{14}O$
2-Ethyl-4-butanol
3-Methylpentanol
RN: 105-30-6 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.284E+01	0	S307	1 1 0 2 2	
1.004E-01	1.025E+01	10.0	S307	1 1 0 2 2	
8.518E-02	8.704E+00	19.6	S307	1 1 0 2 2	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.681E-02	7.848E+00	30.8	S307	1 1 0 2 2	
7.498E-02	7.661E+00	40.3	S307	1 1 0 2 2	
7.295E-02	7.454E+00	50.0	S307	1 1 0 2 2	
7.363E-02	7.523E+00	60.3	S307	1 1 0 2 2	
7.478E-02	7.641E+00	70.1	S307	1 1 0 2 2	
8.133E-02	8.310E+00	80.3	S307	1 1 0 2 2	
8.931E-02	9.126E+00	90.7	S307	1 1 0 2 2	

964. $C_6H_{14}O$

2-Methyl-2-pentanol
Dimethyl-*n*-propylcarbinol
1,1-Dimethyl-1-butanol

RN: 590-36-3 **MP** (°C)**:** –107
MW: 102.18 **BP** (°C)**:** 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.428E-01	3.503E+01	20	G005	1 2 1 1 2	
3.640E-01	3.719E+01	20	H330	0 0 0 0 0	
3.071E-01	3.138E+01	25	G005	1 2 1 1 2	
2.814E-01	2.875E+01	30	G005	1 2 1 1 2	

965. $C_6H_{14}O$

2-Methyl-3-pentanol
i-Propylethylcarbinol

RN: 565-67-3 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.144E-01	2.191E+01	20	G005	1 2 0 0 2	
1.928E-01	1.970E+01	25	G005	1 2 1 1 2	
1.749E-01	1.787E+01	30	G005	1 2 1 1 2	

966. $C_6H_{14}O$

3-Hexanol
n-Propylethylcarbinol
tert-Hexyl alcohol

RN: 623-37-0 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 134.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E-01	2.676E+01	0	S307	1 1 0 2 2	
1.881E-01	1.922E+01	10.1	S307	1 1 0 2 2	
3.062E-01	3.129E+01	20	A015	1 2 1 1 2	
1.683E-01	1.720E+01	20	G005	1 2 1 1 2	
1.608E-01	1.643E+01	20.0	S307	1 1 0 2 2	
1.551E-01	1.584E+01	25	G005	1 2 1 1 2	
1.437E-01	1.468E+01	30	G005	1 2 1 1 2	
1.342E-01	1.371E+01	30.0	S307	1 1 0 2 2	
1.189E-01	1.215E+01	39.8	S307	1 1 0 2 2	
1.065E-01	1.088E+01	50.0	S307	1 1 0 2 2	
9.882E-02	1.010E+01	60.1	S307	1 1 0 2 2	
9.882E-02	1.010E+01	70.2	S307	1 1 0 2 2	
1.036E-01	1.059E+01	80.2	S307	1 1 0 2 2	
1.065E-01	1.088E+01	90.3	S307	1 1 0 2 2	

967. $C_6H_{14}O$
3-Methyl-1-pentanol
3-Methylpentanol
2-Ethyl-4-butanol
RN: 589-35-5 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.190E-02	4.282E+00	25	B060	2 0 1 1 1	

968. $C_6H_{14}O_2$
Acetal
Acetaldehyd-diaethylacetal
Acetaldehyde diethyl acetal
RN: 105-57-7 **MP** (°C)**:**
MW: 118.18 **BP** (°C)**:** 102.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.723E-01	4.400E+01	25	F300	1 0 0 0 1	

969. $C_6H_{14}O_2$
Diethyl cellosolve
Ethylene glycol diethyl ether
1,2-Diethoxyethane
3,6-Dioxaoctane
Ethyl glyme
Diethoxyethane
RN: 629-14-1 **MP** (°C)**:**
MW: 118.18 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.273E-01	2.686E+01	20	D052	1 1 0 0 2	
1.469E+00	1.736E+02	20	M062	1 0 0 0 2	

970. $C_6H_{14}O_3$
Carbitol
2-(2-Ethoxyethoxy)ethanol
RN: 111-90-0 **MP** (°C)**:**
MW: 134.18 **BP** (°C)**:** 196.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E+00	4.843E+02	4.50	C022	1 2 0 0 2	

971. $C_6H_{14}O_6$
D-Mannitol
1,2,3,4,5,6-Hexanehexol
Cordycepic acid
Diosmol
D-Mannite
Manna sugar
RN: 69-65-8 **MP** (°C)**:** 167–170
MW: 182.17 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E+00	2.092E+02	ns	R427	0 0 0 0 0	

972. $C_6H_{14}O_6$
Galactitol
Dulcit
Dulcitol
RN: 608-66-2 **MP** (°C)**:** 189.5
MW: 182.17 **BP** (°C)**:** 277.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.599E-01	2.913E+01	14	D041	1 0 0 0 1	
1.702E-01	3.100E+01	15	F300	1 0 0 0 1	
2.086E+00	3.800E+02	100	F300	1 0 0 0 1	

973. $C_6H_{14}O_6$
Sorbitol
D-Sorbitol
RN: 50-70-4 **MP** (°C)**:** 110
MW: 182.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E+00	6.416E+02	10	M043	1 0 0 0 2	
3.785E+00	6.894E+02	20	M043	1 0 0 0 2	
4.025E+00	7.333E+02	30	M043	1 0 0 0 2	
4.283E+00	7.802E+02	40	M043	1 0 0 0 2	

974. $C_6H_{14}O_6$
Mannitol
D-Mannit
D-Mannitol
RN: 87-78-5 **MP** (°C)**:** 167
MW: 182.17 **BP** (°C)**:** 292

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.081E-01	9.256E+01	0	C073	1 2 2 1 2	
5.171E-01	9.420E+01	0	M043	1 0 0 0 2	

(*continued*)

974. $C_6H_{14}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-01	1.205E+02	10	M043	1 0 0 0 2	
7.734E-01	1.409E+02	15	C073	1 2 2 1 2	
7.740E-01	1.410E+02	15	F300	1 0 0 0 2	
7.408E-01	1.349E+02	18	D041	1 0 0 0 2	
7.936E-01	1.446E+02	19	N051	1 0 2 2 2	
8.609E-01	1.568E+02	20	M043	1 0 0 0 2	
7.571E-01	1.379E+02	21.6	Y412	0 0 0 0 0	
9.762E-01	1.778E+02	25	B106	1 2 2 2 2	
9.732E-01	1.773E+02	25	B106	1 2 2 2 2	
9.739E-01	1.774E+02	25	B106	1 2 2 2 2	
9.639E-01	1.756E+02	25	C073	1 2 2 1 2	
8.255E-01	1.504E+02	25	H087	1 0 2 1 2	
8.373E-01	1.525E+02	26.8	Y412	0 0 0 0 0	
1.000E+00	1.822E+02	30	D011	1 0 1 0 1	
1.105E+00	2.013E+02	30	M043	1 0 0 0 2	
9.149E-01	1.667E+02	30.8	Y412	0 0 0 0 0	
1.254E+00	2.284E+02	35	C073	1 2 2 1 2	
9.899E-01	1.803E+02	35.6	Y412	0 0 0 0 0	
1.062E+00	1.935E+02	38.1	Y412	0 0 0 0 0	
1.411E+00	2.571E+02	40	M043	1 0 0 0 2	
1.133E+00	2.063E+02	41.8	Y412	0 0 0 0 0	
1.760E+00	3.207E+02	50	C073	1 2 2 1 2	
1.827E+00	3.329E+02	51.50	B106	1 2 2 2 2	
2.083E+00	3.794E+02	60	C073	1 2 2 1 2	
2.104E+00	3.833E+02	60	F300	1 0 0 0 2	
2.150E+00	3.917E+02	60	M043	1 0 0 0 2	
2.416E+00	4.401E+02	67.40	B106	1 2 2 2 2	
2.504E+00	4.562E+02	70.50	B106	1 2 2 2 2	
2.936E+00	5.349E+02	80	M043	1 0 0 0 2	
3.015E+00	5.493E+02	82.90	B106	1 2 2 2 2	
3.253E+00	5.927E+02	88.10	B106	1 2 2 2 2	
3.299E+00	6.010E+02	90.10	B106	1 2 2 2 2	
3.590E+00	6.540E+02	98	B106	1 2 2 2 2	
3.628E+00	6.610E+02	99.30	B106	1 2 2 2 2	
3.641E+00	6.633E+02	100	M043	1 0 0 0 2	
8.757E-01	1.595E+02	rt	D021	0 0 1 1 2	

975. $C_6H_{15}N$

Triethylamine
Triaethylamin

RN: 121-44-8 **MP** (°C)**:** –115
MW: 101.19 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E+00	1.799E+02	17.48	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.59	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.64	K142	1 0 0 0 2	

(*continued*)

975. $C_6H_{15}N$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.156E+00	1.170E+02	17.82	K142	1 0 0 0 2	
1.156E+00	1.170E+02	17.85	K142	1 0 0 0 2	
2.791E+00	2.824E+02	18	C088	2 2 2 2 1	
3.434E+00	3.475E+02	18.11	K142	1 0 0 0 2	
3.434E+00	3.475E+02	18.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.13	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.38	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.43	K142	1 0 0 0 2	
1.403E+00	1.420E+02	20	F300	1 0 0 0 2	
6.780E-01	6.861E+01	25.04	V013	2 2 2 2 2	
1.976E-01	2.000E+01	65	F300	1 0 0 0 1	

976. $C_6H_{15}N$
N-Ethyl-*sec*-butylamine
sec-Butylethylamine
2-Butanamine, *N*-ethyl-
2-(Ethylamino)butane
RN: 21035-44-9 **MP** (°C)**:**
MW: 101.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.155E-01	8.253E+01	25	D332	0 0 0 0 0	
6.099E-01	6.172E+01	30	D332	0 0 0 0 0	
4.202E-01	4.252E+01	40	D332	0 0 0 0 0	

977. $C_6H_{15}N$
N-Ethyl-*n*-butylamine
Ethylbutylamine
N-Ethylbutan-1-amine
N-Ethylbutylamine
RN: 13360-63-9 **MP** (°C)**:** –78
MW: 101.19 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	1.015E+02	10	D332	0 0 0 0 0	
5.310E-01	5.373E+01	20	D332	0 0 0 0 0	
3.793E-01	3.838E+01	30	D332	0 0 0 0 0	
2.859E-01	2.893E+01	40	D332	0 0 0 0 0	

978. $C_6H_{15}N$
n-Dipropylamine
Dipropylamine
RN: 142-84-7 **MP** (°C)**:** –63
MW: 101.19 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.470E-01	5.536E+01	12.2	H038	1 2 1 1 2	
2.794E-01	2.828E+01	36.1	H038	1 2 1 1 2	
2.335E-01	2.363E+01	44.1	H038	1 2 1 1 2	
1.900E-01	1.922E+01	52.6	H038	1 2 1 1 2	

979. $C_6H_{15}O_2PS_3$
Thiometon
O,*O*-Dimethyl *S*-(2-ethylmercaptoethyl) dithiophosphate
RN: 640-15-3 **MP** (°C)**:**
MW: 246.35 **BP** (°C)**:** 104

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.118E-04	2.000E-01	20	M061	1 0 0 0 2	
8.118E-04	2.000E-01	25	M161	1 0 0 0 2	

980. $C_6H_{15}O_3PS_2$
Thiolo-methylmercaptophos
Thiolo-methyl demeton
RN: **MP** (°C)**:**
MW: 230.29 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-02	3.300E+00	20	M061	1 0 0 0 2	

981. $C_6H_{15}O_3PS_2$
Thiono-methylmercaptophos
Thiono-methyl demeton
RN: **MP** (°C)**:**
MW: 230.29 **BP** (°C)**:** 74

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-03	3.300E-01	20	M061	1 0 0 0 2	

982. $C_6H_{15}O_4P$
Triethyl phosphate
Ethyl phosphate
Phosphoric acid, triethyl ester
TEP
RN: 78-40-0 **MP** (°C)**:** –56.4
MW: 182.16 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.815E+00	5.128E+02	4.50	C022	1 2 0 0 2	
2.745E+00	5.000E+02	25	F300	1 0 0 0 1	
+2.69E+00	+4.90E+02	ns	S460	0 0 0 0 0	

983. $C_6H_{16}FN_2OP$
Mipafox
N,*N*′-Diisopropylphosphorodiamidic fluoride
RN: 371-86-8 **MP** (°C)**:** 65
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.066E-01	7.407E+01	ns	M061	0 0 0 0 0	

984. $C_6H_{16}N_2$
1,6-Hexanediamine
Hexamethylenediamine
RN: 124-09-4 **MP** (°C)**:** 42
MW: 116.21 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E+00	7.115E+02	4.50	C022	1 2 0 0 2	

985. $C_6H_{17}N_3O_{10}S$
Glycine sulfate
Triglycine sulfate
RN: 513-29-1 **MP** (°C)**:**
MW: 323.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.314E-01	1.071E+02	0	M043	1 0 0 0 1	
5.155E-01	1.667E+02	10	M043	1 0 0 0 1	
6.576E-01	2.126E+02	20	M043	1 0 0 0 1	
8.188E-01	2.647E+02	30	M043	1 0 0 0 1	
9.600E-01	3.103E+02	40	M043	1 0 0 0 1	
1.326E+00	4.286E+02	60	M043	1 0 0 0 1	

986. $C_6H_{18}N_4$
Triethylenetetramine
N,*N*′-bis(2-Aminoethyl)-ethylenediamine
1,8-Diamino-3,6-diazaoctane
1,4,7,10-Tetraazadecane
3,6-Diazaoctane-1,8-diamine
Trientine
RN: 112-24-3 **MP** (°C)**:** 12
MW: 146.24 **BP** (°C)**:** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.655E+00	8.269E+02	4.50	C022	1 2 0 0 2	

987. C_6Br_6
Hexabromobenzene
RN: 87-82-1 **MP** (°C)**:** 327
MW: 551.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.558E-11	4.720E-08	10	K440	0 0 0 0 0	
1.994E-10	1.100E-07	25	K440	0 0 0 0 0	
4.207E-10	2.320E-07	35	K440	0 0 0 0 0	

988. $C_6Cl_4O_2$
Chloranil
Tetrachloro-*p*-benzoquinone
2,3,5,6-Tetrachloro-*p*-benzoquinone
2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione
Vulklor
Coversan
RN: 118-75-2 **MP** (°C)**:** 290
MW: 245.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-03	2.500E-01	rt	M161	0 0 0 0 2	

989. $C_6Cl_5NO_2$
Quintozene
Pentachloronitrobenzene
Avical
Eorthcicle
Quintobenzene
RN: 82-68-8 **MP** (°C)**:** >139
MW: 295.34 **BP** (°C)**:** 328

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.430E-04	20	E308	1 2 2 1 1	
1.862E-06	5.500E-04	22	K137	1 1 2 1 0	
1.490E-06	4.400E-04	22.5	G301	0 0 0 0 0	

990. C_6Cl_6
Hexachlorobenzene
Benzene hexachloride
HCB
Hexa-chlorobenzene
RN: 118-74-1 **MP** (°C)**:** 228
MW: 284.78 **BP** (°C)**:** 324.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.585E-05	20	B179	0 0 0 0 0	
1.721E-08	4.900E-06	20	C113	1 0 1 1 1	
2.598E-08	7.400E-06	20	H300	1 1 2 2 1	
1.896E-08	5.400E-06	20	H300	1 1 2 2 1	
2.042E-08	5.815E-06	20	K337	1 0 0 0 2	
1.380E-08	3.931E-06	22	K305	1 0 1 1 2	
1.756E-08	5.000E-06	22.5	G301	0 0 0 0 0	
1.700E-08	4.841E-06	25	B317	0 0 0 0 0	
1.650E-08	4.699E-06	25	M342	1 0 1 1 2	
2.107E-08	6.000E-06	26.70	L095	2 2 1 1 2	
<3.51E-06	<1.00E-03	30	M311	1 1 2 2 0	
7.023E-08	2.000E-05	ns	L072	0 0 0 0 1	
2.107E-08	6.000E-06	ns	L311	0 0 0 0 1	
1.650E-07	4.699E-05	ns	M308	0 0 1 1 2	
2.458E-05	7.000E-03	rt	H053	0 2 2 2 0	γ isomer

991. C_6F_6
Hexafluorobenzene
Perfluorobenzene
RN: 392-56-3 **MP** (°C)**:** 3.9 C
MW: 186.06 **BP** (°C)**:** 81 C at 743 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-03	7.788E-01	8.30	F418	0 0 0 0 0	
3.598E-03	6.694E-01	18.20	F418	0 0 0 0 0	
3.315E-03	6.167E-01	27.81	F418	0 0 0 0 0	
3.198E-03	5.950E-01	37.66	F418	0 0 0 0 0	
3.148E-03	5.857E-01	47.35	F418	0 0 0 0 0	
3.209E-03	5.971E-01	56.61	F418	0 0 0 0 0	
3.420E-03	6.363E-01	66.60	F418	0 0 0 0 0	

992. $C_7H_3Br_2NO$
Bromoxynil
3,5-Dibromo-4-hydroxybenzonitrile
4-Cyano-2,6-dibromophenol
RN: 1689-84-5 **MP** (°C)**:** 190
MW: 276.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.694E-04	1.300E-01	25	M161	1 0 0 0 2	
4.694E-04	1.300E-01	ns	M061	0 0 0 0 2	

993. $C_7H_3Br_3O_2$
2,4,6-Tribromobenzoic acid
2,4,6-Tribrom-benzoesaeure
RN: 633-12-5 **MP** (°C)**:**
MW: 358.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.754E-03	3.500E+00	15	F300	1 0 0 0 1	
1.533E-02	5.500E+00	100	F300	1 0 0 0 1	

994. $C_7H_3Cl_2N$
Dichlobenil
2,6-Dichlorobenzonitrile
Benzonitrile, 2,6-dichloro-
RN: 1194-65-6 **MP** (°C)**:** 145
MW: 172.01 **BP** (°C)**:** 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.046E-04	1.800E-02	20	B185	0 0 0 0 0	
1.046E-04	1.800E-02	20	B200	1 0 0 1 1	
1.046E-04	1.800E-02	20	G319	0 0 0 0 0	
1.046E-04	1.800E-02	20	M161	1 0 0 0 1	
1.163E-04	2.000E-02	25	B185	0 0 0 0 0	
5.813E-05	1.000E-02	25	M061	1 0 0 0 1	
1.046E-04	1.800E-02	ns	V303	0 0 0 0 1	

995. $C_7H_3Cl_3O_2$
2,3,6-Trichlorobenzoic acid
2,3,6-TBA
RN: 50-31-7 **MP** (°C)**:** 125
MW: 225.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.726E-02	8.400E+00	20	B200	1 0 0 0 1	
3.415E-02	7.700E+00	22	M161	1 0 0 0 1	

996. $C_7H_3Cl_5O$
Pentachlorbenzyl alcohol
Blastin
PCBA
RN: 16022-69-8 **MP** (°C)**:**
MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.134E-07	2.000E-04	25	M061	0 0 0 0 0	

997. $C_7H_3I_2NO$
Ioxynil
4-Cyano-2,6-diiodophenol
4-Hydroxy-3,5-diiodobenzonitrile
RN: 1689-83-4 **MP** (°C)**:** 212
MW: 370.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.348E-04	5.000E-02	20	F311	1 2 2 2 1	
3.505E-04	1.300E-01	25	B200	1 0 0 0 2	
1.348E-04	5.000E-02	25	M161	1 0 0 0 1	

998. $C_7H_3N_3O_8$
2,4,6-Trinitrobenzoic acid
2,4,6-Trinitrobenzoesaeure
Acide 2,4,6-trinitrobenzoique
RN: 129-66-8 **MP** (°C)**:** 228.7
MW: 257.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-02	2.010E+01	23	F300	1 0 0 0 2	
7.824E-02	2.012E+01	23.5	D067	1 2 0 0 2	
1.560E-01	4.012E+01	50	D067	1 2 0 0 2	
1.560E-01	4.010E+01	50	F300	1 0 0 0 2	

999. C_7H_4BrN
4-Bromobenzonitrile
p-Bromobenzonitrile
4-Bromobenzoic acid nitrile
RN: 623-00-7 **MP** (°C)**:** 111 C
MW: 182.03 **BP** (°C)**:** 236 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.635E-04	1.572E-01	22	J420	0 0 0 0 0	pH 6.5

1000. $C_7H_4BrNO_4$
3-Bromo-2-nitrobenzoic acid
Benzoic acid, 3-bromo-2-nitro-
RN: 116529-61-4 **MP** (°C)**:**
MW: 246.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.012E-02	7.410E+00	25	H089	1 2 0 0 2	
1.341E-03	3.300E-01	25	H089	1 2 0 0 1	

1001. C_7H_4BrNS
4-Bromophenyl isothiocyanate
1-Bromo-4-isothiocyanato-benzene
RN: 1985-12-2 **MP** (°C)**:** 60.5
MW: 214.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	1.156E-02	25	D019	1 1 1 1 1	

1002. C_7H_4BrNS
3-Bromophenyl isothiocyanate
1-Bromo-3-isothiocyanato-benzene
RN: 2131-59-1 **MP** (°C)**:**
MW: 214.09 **BP** (°C)**:** 256.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	2.441E-02	25	D019	1 1 1 1 2	
8.200E-05	1.756E-02	25	K032	2 2 0 1 1	

1003. $C_7H_4ClNO_4$
3-Chloro-2-nitrobenzoic acid
2-Nitro-3-chlorobenzoic acid
RN: 4771-47-5 **MP** (°C)**:**
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.332E-03	4.700E-01	25	H089	1 2 0 0 1	

1004. $C_7H_4ClNO_4$
4-Chloro-3-nitrobenzoic acid
3-Nitro-4-chlorobenzoic acid
RN: 96-99-1 **MP** (°C)**:** 181
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	3.427E-01	ns	C014	0 0 0 1 1	

1005. $C_7H_4ClNO_4$
5-Chloro-2-nitrobenzoic acid
2-Nitro-5-chlorobenzoic acid
RN: 2516-95-2 **MP** (°C)**:**
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-02	9.670E+00	25	H089	1 2 0 0 2	

1006. C_7H_4ClNS
3-Chlorophenyl isothiocyanate
1-Chloro-3-isothiocyanato-benzene
RN: 2392-68-9 **MP** (°C)**:**
MW: 169.63 **BP** (°C)**:** 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.393E-02	25	D019	1 1 1 1 0	
1.120E-04	1.900E-02	25	K032	2 2 0 1 2	

1007. $C_7H_4Cl_2O_2$
3,5-Dichlorobenzoic acid
Benzoic acid, 3,5-dichloro-
RN: 51-36-5 **MP** (°C)**:** 186
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-04	1.471E-01	ns	C014	0 0 0 1 1	

1008. $C_7H_4Cl_2O_2$
2,6-Dichlorobenzoic acid
2,6-Dichlor-benzoesaeure
RN: 50-30-6 **MP** (°C)**:**
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.414E+01	ns	C014	0 0 0 1 1	

1009. $C_7H_4Cl_2O_2$
2,4-Dichlorobenzoic acid
2,4-Dichlor-benzoesaeure
RN: 50-84-0 **MP** (°C)**:**
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.775E-01	ns	C014	0 2 0 1 1	

1010. $C_7H_4Cl_2O_2$
3,4-Dichlorobenzoic acid
Benzoic acid, 3,4-dichloro-
RN: 51-44-5 **MP** (°C)**:** 208
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	6.112E-02	ns	C014	0 0 0 1 1	

1011. $C_7H_4Cl_3NO_3$
Triclopyr
Garlon
(3,5,6-Trichloro-2-pyridinyl)oxyacetic acid
Crossbow turflon
RN: 55335-06-3 **MP** (°C)**:** 149
MW: 256.47 **BP** (°C)**:** 290

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.300E-01	ns	K138	0 0 0 0 1	

1012. $C_7H_4Cl_4O$
2,4,5,6-Tetrachloro-3-methyl-phenol
m-Cresol, 2,4,5,6-tetrachloro-
Phenol, 2,3,4,6-tetrachloro-5-methyl-
RN: 10460-33-0 **MP** (°C)**:**
MW: 245.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.148E-03	25	B316	0 0 0 0 0	

1013. $C_7H_4Cl_4O$
2,3,4,5-Tetrachloroanisole
Benzene, 1,2,3,4-tetrachloro-5-methoxy-
Anisole, 2,3,4,5-tetrachloro-
RN: 938-86-3 **MP** (°C)**:** 88
MW: 245.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.490E-06	1.350E-03	25	L348	1 2 2 1 2	

1014. C_7H_4INS
4-Iodophenyl isothiocyanate
4-Iodophenylisothiocyanate
RN: 2059-76-9 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.350E-02	25	D019	1 1 1 1 1	

1015. C_7H_4INS

3-Iodophenyl isothiocyanate
m-Iodophenyl isothiocyanate
RN: 3125-73-3 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.483E-03	25	K032	2 2 0 1 0	

1016. $C_7H_4I_2O_3$

3,5-Diiodosalicylic acid
2-Hydroxy-3,5-diiod-benzoesaeure
RN: 133-91-5 **MP** (°C)**:** 235.5
MW: 389.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.274E-04	1.666E-01	10	C072	1 2 1 1 2	
1.795E-03	7.000E-01	15	F300	1 0 0 0 1	
4.931E-04	1.923E-01	25	C072	1 2 1 1 2	
3.847E-03	1.500E+00	h	F300	1 0 0 0 1	

1017. $C_7H_4N_2O_2S$

3-Nitrophenyl isothiocyanate
m-Nitrophenylisothiocyanate
RN: 3529-82-6 **MP** (°C)**:**
MW: 180.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-04	5.045E-02	25	K032	2 2 0 1 2	

1018. $C_7H_4N_2O_6$

2,4-Dinitrobenzoic acid
2,4-Dinitrobenzoesaeure
RN: 610-30-0 **MP** (°C)**:**
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.580E-02	1.820E+01	25	F300	1 0 0 0 2	
4.900E-02	1.039E+01	ns	C014	0 0 0 1 1	

1019. $C_7H_4N_2O_6$
2,6-Dinitrobenzoic acid
2,6-Dinitrobenzoesaeure
RN: 603-12-3 **MP** (°C)**:**
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	1.612E+01	ns	C014	0 2 0 1 1	

1020. $C_7H_4N_2O_6$
3,4-Dinitrobenzoic acid
3,4-Dinitrobenzoesaeure
RN: 528-45-0 **MP** (°C)**:** 166
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-02	6.700E+00	25	F300	1 0 0 0 1	

1021. $C_7H_4N_2O_6$
3,5-Dinitrobenzoic acid
3,5-Dinitrobenzoesaeure
RN: 99-34-3 **MP** (°C)**:** 205
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.347E+00	25	K040	1 0 2 1 2	
2.923E-03	6.200E-01	25	P037	2 0 1 1 1	

1022. $C_7H_4N_4O_9$
2,3,5,6-Tetranitroanisol
RN: **MP** (°C)**:**
MW: 288.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.941E-04	2.000E-01	50	F300	1 0 0 0 0	
4.165E-03	1.200E+00	100	F300	1 0 0 0 1	

1023. $C_7H_4O_6$
Chelidonic acid
Chelidonsaeure
RN: 99-32-1 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.767E-02	1.430E+01	25	F300	1 0 0 0 2	
2.064E-01	3.800E+01	100	F300	1 0 0 0 1	

1024. $C_7H_4O_7$
Meconic acid
Mekonsaeure
RN: 497-59-6 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.198E-02	8.400E+00	25	F300	1 0 0 0 1	
1.034E+00	2.070E+02	100	F300	1 0 0 0 2	

1025. $C_7H_5BrO_2$
p-Bromobenzoic acid
4-Bromobenzoic acid
RN: 586-76-5 **MP** (°C)**:** 252.0
MW: 201.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-04	5.600E-02	22.5	G301	0 0 0 0 0	
2.985E-04	6.000E-02	ns	B150	0 0 2 2 1	
2.885E-04	5.800E-02	ns	B150	0 0 2 2 1	
2.800E-04	5.629E-02	ns	C014	0 0 0 1 1	

1026. $C_7H_5BrO_2$
m-Bromobenzoic acid
3-Bromobenzoic acid
RN: 585-76-2 **MP** (°C)**:** 155
MW: 201.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.021E-01	ns	C014	0 0 0 1 1	

1027. $C_7H_5ClN_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(chloroacetyl)-1,5-dihydro-
RN: 96448-62-3 **MP** (°C)**:**
MW: 212.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.174E-04	1.100E-01	22	B428	1 2 1 2 1	

1028. $C_7H_5ClO_2$

meta-Chlorobenzoic acid
3-Chlorobenzoic acid
m-Chlorobenzoic acid
3-Chlor-benzoesaeure

RN: 535-80-8 **MP** (°C)**:** 154
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-04	4.000E-02	0	F300	1 0 0 0 0	
4.080E-03	6.388E-01	24.99	B391	0 0 0 0 0	
2.555E-03	4.000E-01	25	F300	1 0 0 0 0	
2.543E-03	3.982E-01	25	T066	1 0 0 0 2	
2.555E-03	4.000E-01	37	M360	1 2 1 1 2	
2.460E-03	3.852E-01	ns	O004	0 2 1 1 2	

1029. $C_7H_5ClO_2$

p-Chlorobenzoic acid
4-Chlorobenzoic acid
Chloradracylic
4-Chlor-benzoesaeure

RN: 74-11-3 **MP** (°C)**:** 235
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-04	9.000E-02	22.5	G301	0 0 0 0 0	
8.000E-04	1.253E-01	24.99	B391	0 0 0 0 0	
7.026E-04	1.100E-01	25	C410	2 0 2 2 1	
4.918E-04	7.700E-02	25	F300	1 0 0 0 1	
4.639E-04	7.263E-02	25	T066	1 0 0 0 2	
7.026E-04	1.100E-01	37	M360	1 2 1 1 2	
4.918E-04	7.700E-02	ns	B150	0 0 2 2 1	
4.350E-04	6.811E-02	ns	O004	0 2 1 1 2	

1030. $C_7H_5ClO_2$

o-Chlorobenzoic acid
2-Chlor-benzoesaeure
2-Chlorobenzoic acid

RN: 118-91-2 **MP** (°C)**:** 142
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.288E+00	24.99	B391	0 0 0 0 0	
1.916E-02	3.000E+00	25	C410	2 0 2 2 1	
1.341E-02	2.100E+00	25	F300	1 0 0 0 1	
8.686E-03	1.360E+00	25	P037	2 0 1 1 2	
1.865E-02	2.920E+00	37	M360	1 2 1 1 2	
2.574E-01	4.030E+01	100	F300	1 0 0 0 2	
1.330E-02	2.082E+00	ns	C014	0 0 0 1 2	
1.362E-02	2.132E+00	ns	O004	0 2 1 1 2	

1031. $C_7H_5Cl_2NO$
2,6-Dichlorobenzamide
Dichlorobenzamide
BAM
RN: 2008-58-4 **MP** (°C)**:** 198
MW: 190.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E-02	2.700E+00	22.5	G301	0 0 0 0 0	

1032. $C_7H_5Cl_2NO_2$
Chloramben
3-Amino-2,5-dichlorobenzoic acid
RN: 133-90-4 **MP** (°C)**:** 201
MW: 206.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-03	7.000E-01	25	B200	1 0 0 0 2	
3.398E-03	7.000E-01	25	M161	1 0 0 0 2	
3.398E-03	7.000E-01	ns	B185	0 0 0 0 0	

1033. $C_7H_5Cl_2NS$
2,6-Dichlorothiobenzamide
Prefix
Chlorthiamid
RN: 1918-13-4 **MP** (°C)**:** 151.5
MW: 206.09 **BP** (°C)**:** 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.561E-03	9.400E-01	20	M061	1 0 0 0 2	
4.610E-03	9.500E-01	21	M161	1 0 0 0 2	

1034. $C_7H_5Cl_3O$
2,3,4-Trichloroanisole
1,2,3-Trichloro-4-methoxy-benzene
RN: 54135-80-7 **MP** (°C)**:** 70
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.107E-05	1.080E-02	25	L348	1 2 2 1 2	

1035. $C_7H_5Cl_3O$

2,4,6-Trichloro-3-methylphenol
m-Cresol, 2,4,6-trichloro-
2,4,6-Trichloro-*m*-cresol
RN: 551-76-8 **MP** (°C)**:**
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.121E-01	25	B316	0 0 0 0 0	

1036. $C_7H_5Cl_3O$

2,4,6-Trichloroanisole
1-Methoxy-2,4,6-trichlorobenzene
Methyl 2,4,6-trichlorophenyl ether
Tyrene
RN: 87-40-1 **MP** (°C)**:** 61
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-05	1.320E-02	25	L348	1 2 2 1 2	

1037. $C_7H_5FO_2$

m-Fluorobenzoic acid
3-Fluor-benzoesaeure
3-Fluorobenzoic acid
RN: 455-38-9 **MP** (°C)**:** 123
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.071E-02	1.500E+00	25	F300	1 0 0 0 1	

1038. $C_7H_5FO_2$

o-Fluorobenzoic acid
2-Fluorobenzoic acid
RN: 445-29-4 **MP** (°C)**:** 123
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-02	7.200E+00	25	F300	1 0 0 0 1	
5.129E-02	7.186E+00	ns	R427	0 0 0 0 0	

1039. $C_7H_5FO_2$
p-Fluorobenzoic acid
4-Fluor-benzoesaeure
4-Fluorobenzoic acid
RN: 456-22-4 **MP** (°C)**:** 182.6
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.564E-03	1.200E+00	25	F300	1 0 0 0 1	

1040. $C_7H_5F_3N_2O_4S$
3-Trifluoromethyl-4-nitrobenzenesulfonamide
4-Nitro-3-(trifluoromethyl)benzenesulfonamide
RN: 21988-05-6 **MP** (°C)**:**
MW: 270.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-04	1.756E-01	15	K024	1 2 1 1 2	

1041. $C_7H_5IO_2$
p-Iodobenzoic acid
4-Iodobenzoic acid
RN: 619-58-9 **MP** (°C)**:**
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	2.778E-02	15	D008	1 0 1 1 2	intrinsic

1042. $C_7H_5IO_2$
o-Iodobenzoic acid
2-Iodobenzoic acid
RN: 88-67-5 **MP** (°C)**:** 162
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.860E-03	4.613E-01	15	D008	1 0 1 1 2	0.002N HCl

1043. $C_7H_5IO_2$
m-Iodobenzoic acid
3-Iodobenzoic acid
RN: 618-51-9 **MP** (°C)**:** 187
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-04	1.334E-01	15	D008	1 0 1 1 2	0.002N HCl

1044. $C_7H_5I_2NO_3$
3,5-Diiodo-4-pyridone-*N*-acetic acid
3,5-Diiod-pyridon-(4)-*N*-essigsaeure
3,5-Diiodo-4-pyridone-1-acetic acid
Diodon
1,4-Dihydro-3,5-diiodo-4-oxopyridine-1-acetic acid
RN: 101-29-1 **MP** (°C)**:** 244
MW: 404.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.883E-03	2.787E+00	ns	H055	0 0 0 0 0	

1045. C_7H_5N
Benzonitrile
Benzonitril
Benzenenitrile
Benzoic acid nitrile
Phenyl cyanide
Cyanobenzene
RN: 100-47-0 **MP** (°C)**:** –13
MW: 103.12 **BP** (°C)**:** 190.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.839E-02	1.896E+00	24.0	P321	0 0 0 0 0	
4.200E-02	4.331E+00	25	M327	1 0 0 1 2	
3.671E-02	3.786E+00	35.5	P321	0 0 0 0 0	
5.400E-02	5.569E+00	50.0	P321	0 0 0 0 0	
4.056E-02	4.182E+00	57.0	P321	0 0 0 0 0	
5.496E-02	5.668E+00	62.5	P321	0 0 0 0 0	
8.268E-02	8.527E+00	85.0	P321	0 0 0 0 0	
8.459E-02	8.723E+00	90.5	P321	0 0 0 0 0	
9.981E-02	1.029E+01	95.5	P321	0 0 0 0 0	
9.697E-02	1.000E+01	100	F300	1 0 0 0 0	
1.065E-01	1.098E+01	101.0	P321	0 0 0 0 0	
1.339E-01	1.381E+01	116.0	P321	0 0 0 0 0	
1.920E-01	1.980E+01	127.5	P321	0 0 0 0 0	
2.171E-01	2.239E+01	142.0	P321	0 0 0 0 0	
2.888E-01	2.979E+01	148.0	P321	0 0 0 0 0	
2.834E-01	2.922E+01	149.0	P321	0 0 0 0 0	
3.873E-01	3.994E+01	160.5	P321	0 0 0 0 0	
5.747E-01	5.927E+01	164.5	P321	0 0 0 0 0	
1.373E+00	1.416E+02	201.0	P321	0 0 0 0 0	
2.937E+00	3.029E+02	211.0	P321	0 0 0 0 0	
9.696E-04	9.999E-02	ns	L055	0 0 0 0 1	

1046. C_7H_5NOS

4-Hydroxyphenyl isothiocyanate
4-Hydroxyphenylisothiocyanate
RN: 2131-60-4 **MP** (°C)**:**
MW: 151.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.150E-03	3.251E-01	25	D019	1 1 1 1 2	

1047. C_7H_5NOS

3-Hydroxyphenyl isothiocyanate
m-Hydroxyphenyl isothiocyanate
RN: 3125-63-1 **MP** (°C)**:**
MW: 151.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.542E+00	25	K032	2 2 0 1 2	
1.023E-02	1.547E+00	ns	R427	0 0 0 0 0	

1048. $C_7H_5NO_3$

m-Nitrobenzaldehyde
3-Nitrobenzaldehyde
3-Nitro-benzaldehyd
RN: 99-61-6 **MP** (°C)**:** 58
MW: 151.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.617E-05	1.000E-02	25	F300	1 0 0 0 1	
3.309E+00	5.000E+02	58.0	S118	1 2 0 1 0	
6.292E-02	9.509E+00	75.1	S118	1 2 0 1 1	
3.272E+00	4.945E+02	85.2	S118	1 2 0 1 2	
1.266E-01	1.913E+01	111.9	S118	1 2 0 1 2	
1.934E-01	2.922E+01	136.4	S118	1 2 0 1 2	
3.103E-01	4.689E+01	157.3	S118	1 2 0 1 2	
6.293E-01	9.510E+01	181.0	S118	1 2 0 1 2	
8.142E-01	1.230E+02	191.4	S118	1 2 0 1 2	
1.253E+00	1.893E+02	205.4	S118	1 2 0 1 2	
1.878E+00	2.838E+02	211.8	S118	1 2 0 1 2	

1049. $C_7H_5NO_3$
o-Nitrobenzaldehyde
2-Nitrobenzaldehyde
2-Nitro-benzaldehyd
RN: 552-89-6 **MP** (°C)**:** 44
MW: 151.12 **BP** (°C)**:** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-04	2.000E-02	25	F300	1 0 0 0 1	
4.600E-02	6.951E+00	66.9	S118	1 2 0 1 1	
9.972E-02	1.507E+01	103.1	S118	1 2 0 1 1	
3.001E-01	4.535E+01	166.0	S118	1 2 0 1 1	

1050. $C_7H_5NO_3$
p-Nitrobenzaldehyde
4-Nitrobenzaldehyde
RN: 555-16-8 **MP** (°C)**:** 106.5
MW: 151.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.871E-01	2.828E+01	132.4	S118	1 2 0 1 2	
5.341E-01	8.071E+01	176.5	S118	1 2 0 1 2	
1.133E+00	1.713E+02	205.4	S118	1 2 0 1 2	
1.814E+00	2.742E+02	215.5	S118	1 2 0 1 2	

1051. $C_7H_5NO_3S$
Saccharin
1,1-Dioxide-1,2-benzisothiazol-3-(2H)-one
3-Benzisothiazolinone 1,1-dioxide
1,2-Benzisothiazol-3(2H)-one-1,1-dioxide
Kandiset
Glucid
RN: 81-07-2 **MP** (°C)**:** 228.8
MW: 183.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-02	4.300E+00	25	F300	1 0 0 0 1	
1.880E-01	3.444E+01	30	M015	1 0 2 1 0	EFG

1052. $C_7H_5NO_4$
Quinolinic acid
2,3-Pyridinedicarboxylic acid
Pyridine-2,3-dicarboxylic acid
Pyridine-2,3-dicarboxylate
RN: 89-00-9 **MP** (°C)**:** 190
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	5.500E+00	7	F300	1 0 0 0 1	
6.600E-02	1.103E+01	25	C104	2 2 1 1 2	
6.400E-02	1.070E+01	25	C104	2 2 1 1 2	

1053. $C_7H_5NO_4$
p-Nitrobenzoic acid
4-Nitrobenzoic acid
RN: 62-23-7 **MP** (°C)**:** 242.4
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-03	2.000E-01	15	F300	1 0 0 0 2	
2.525E-03	4.220E-01	24.99	B391	0 0 0 0 0	
1.660E-03	2.774E-01	25	H071	2 2 2 1 2	
3.471E-03	5.800E-01	37	B171	2 0 1 1 2	

1054. $C_7H_5NO_4$
o-Nitrobenzoic acid
2-Nitrobenzoic acid
RN: 552-16-9 **MP** (°C)**:** 147.5
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-02	6.551E+00	18	D058	1 0 1 1 2	
3.340E-02	5.582E+00	24.99	B391	0 0 0 0 0	
4.325E-02	7.228E+00	25	D058	1 0 1 1 2	
4.488E-02	7.500E+00	25	F300	1 0 0 0 1	
4.350E-02	7.270E+00	25	H071	2 2 2 1 2	
4.700E-02	7.855E+00	25	K040	1 0 2 1 2	
4.360E-02	7.287E+00	25	K053	2 2 2 2 2	
4.430E-02	7.404E+00	25	L050	2 0 1 2 2	
4.415E-02	7.378E+00	25	R016	0 0 0 0 0	
4.700E-02	7.855E+00	26.4	P043	2 0 1 1 2	

1055. $C_7H_5NO_4$
m-Nitrobenzoic acid
3-Nitrobenzoic acid
RN: 121-92-6 **MP** (°C)**:** 142.0
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.436E-02	2.400E+00	15	F300	1 0 0 0 1	
1.530E-02	2.557E+00	24.99	B391	0 0 0 0 0	
2.121E-02	3.545E+00	25	C076	0 0 0 0 0	
2.140E-02	3.576E+00	25	K040	1 0 2 1 2	
1.227E-02	2.050E+00	25	P037	2 0 1 1 2	
6.582E-02	1.100E+01	37	B171	2 0 1 1 2	
2.334E-02	3.900E+00	ns	B361	0 0 0 0 0	

1056. $C_7H_5NO_4$
Isocinchomeronic acid
2,5-Pyridinedicarboxylic acid
Pyridine-2,5-dicarboxylic acid
RN: 100-26-5 **MP** (°C)**:** 254
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.237E+00	25	C104	2 2 1 1 2	
7.100E-03	1.187E+00	25	C104	2 2 1 1 2	

1057. $C_7H_5NO_4$
Cinchomeronic acid
3,4-Pyridinedicarboxylic acid
RN: 490-11-9 **MP** (°C)**:** 256
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	2.340E+00	25	C104	2 2 1 1 2	
1.380E-02	2.306E+00	25	C104	2 2 1 1 2	

1058. $C_7H_5NO_4$
3,5-Pyridinedicarboxylic acid
Dinicotinic acid
RN: 499-81-0 **MP** (°C)**:**
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.070E+00	25	C104	2 2 1 1 2	

1059. $C_7H_5NO_4$
4-Formyl-2-NO2-phenol
RN: **MP** (°C)**:**
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.122E-03	1.875E-01	ns	R424	0 0 0 0 0	

1060. $C_7H_5NO_4$
Lutidinic acid
2,4-Pyridinedicarboxylic acid
RN: 499-80-9 **MP** (°C)**:** 248
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-02	2.490E+00	25	C104	2 2 1 1 2	
1.480E-02	2.473E+00	25	C104	2 2 1 1 2	

1061. $C_7H_5NO_5$
3-Nitrosalicylic acid
3-Nitro-salicylsaeure
RN: 85-38-1 **MP** (°C)**:** 128
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.099E-03	1.300E+00	16	F300	1 0 0 0 1	

1062. $C_7H_5NO_5$
5-Nitrosalicylic acid
5-Nitrosalicylsaeure
RN: 96-97-9 **MP** (°C)**:** 229–230
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-02	2.000E+00	45	F300	1 0 0 0 0	

1063. C_7H_5NS
Benzothiazole
Benzthiazol
RN: 95-16-9 **MP** (°C)**:** 2
MW: 135.19 **BP** (°C)**:** 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	4.275E+00	ns	S460	0 0 0 0 0	

1064. C_7H_5NS
Phenyl isothiocyanate
Isothiocyanatobenzene
Phenyl mustard oil
PITC
RN: 103-72-0 **MP** (°C)**:** –21.0
MW: 135.19 **BP** (°C)**:** 221.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-04	8.990E-02	25	D019	1 1 1 1 2	

1065. $C_7H_5N_3O_6$
2,4,6-Trinitrotoluene
2,4,6-Tronitrotoluol
RN: 118-96-7 **MP** (°C)**:** 80.1
MW: 227.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-04	1.100E-01	.3	D065	1 2 2 1 2	
4.842E-04	1.100E-01	.3	T020	1 2 2 2 2	
4.843E-04	1.100E-01	.30	F300	1 0 0 0 1	
4.975E-04	1.130E-01	5.9	D065	1 2 2 1 2	
4.974E-04	1.130E-01	5.9	T020	1 2 2 2 2	
5.283E-04	1.200E-01	20	D065	1 2 2 1 2	
5.283E-04	1.200E-01	20.0	T020	1 2 2 2 2	
8.937E-04	2.030E-01	33.1	D065	1 2 2 1 2	
8.936E-04	2.030E-01	33.1	T020	1 2 2 2 2	
1.497E-03	3.400E-01	44.2	D065	1 2 2 1 2	
1.496E-03	3.399E-01	44.2	T020	1 2 2 2 2	
1.629E-03	3.700E-01	45	D065	1 2 2 1 2	
1.628E-03	3.699E-01	45.0	T020	1 2 2 2 2	
2.351E-03	5.340E-01	53	D065	1 2 2 1 2	
2.350E-03	5.337E-01	53.0	T020	1 2 2 2 2	
2.703E-03	6.140E-01	57.1	D065	1 2 2 1 2	
2.702E-03	6.136E-01	57.1	T020	1 2 2 2 2	
4.240E-03	9.630E-01	73.2	D065	1 2 2 1 2	
4.236E-03	9.621E-01	73.2	T020	1 2 2 2 2	
6.054E-03	1.375E+00	94.4	D065	1 2 2 1 2	
6.045E-03	1.373E+00	94.4	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.5	D065	1 2 2 1 2	
6.449E-03	1.465E+00	99.5	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.50	F300	1 0 0 0 2	
6.026E-04	1.369E-01	ns	R427	0 0 0 0 0	

1066. $C_7H_5N_3O_7$
2,4,6-Trinitro-*m*-cresol
2,4,6-Trinitro-*m*-kresol
RN: 3238-38-8 **MP** (°C)**:**
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.226E-03	2.000E+00	15	F300	1 0 0 0 0	

1067. $C_7H_5N_3O_7$
Methyl picric acid
2,4,6-Trinitro-3-methylphenol
3-Methyl-2,4,6-trinitrophenol
2,4,6-Trinitro-*m*-cresol
RN: 602-99-3 **MP** (°C)**:**
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	2.431E+00	25	K053	2 2 2 2 2	

1068. $C_7H_5N_3O_7$
2,4,6-Trinitroanisole
2-Methoxy-1,3,5-trinitro-benzene
Methyl picrate
RN: 606-35-9 **MP** (°C)**:** 69
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.224E-04	2.000E-01	15	D079	1 2 0 0 1	
5.627E-03	1.368E+00	50	D079	1 2 0 0 2	
1.594E-02	3.875E+00	100	D079	1 2 0 0 2	

1069. $C_7H_5N_5O_8$
Nitramine
Tetryl
N-Methyl-*N*,2,4,5-tetranitroaniline
RN: 479-45-8 **MP** (°C)**:** 131
MW: 287.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.776E-04	5.100E-02	.5	T015	1 2 0 1 1	
1.776E-04	5.100E-02	.50	D066	1 2 2 1 2	
1.741E-04	5.000E-02	.50	F300	1 0 0 0 0	
2.403E-04	6.900E-02	9.6	D066	1 2 2 1 2	
2.403E-04	6.900E-02	9.6	T015	1 2 0 1 1	
2.473E-04	7.100E-02	14.8	D066	1 2 2 1 1	

(*continued*)

1069. $C_7H_5N_5O_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-04	7.099E-02	14.8	T015	1 2 0 1 1	
2.577E-04	7.400E-02	20.5	D066	1 2 2 1 1	
2.577E-04	7.399E-02	20.5	T015	1 2 0 1 1	
2.925E-04	8.400E-02	30	D066	1 2 2 1 1	
2.925E-04	8.399E-02	30.0	T015	1 2 0 1 1	
3.274E-04	9.400E-02	35	D066	1 2 2 1 1	
3.273E-04	9.399E-02	35.0	T015	1 2 0 1 1	
3.726E-04	1.070E-01	40	D066	1 2 2 1 2	
3.726E-04	1.070E-01	40.0	T015	1 2 0 1 2	
4.701E-04	1.350E-01	45	D066	1 2 2 1 2	
4.701E-04	1.350E-01	45.0	T015	1 2 0 1 2	
6.965E-04	2.000E-01	50	D066	1 2 2 1 2	
6.964E-04	2.000E-01	50.0	T015	1 2 0 1 2	
1.219E-03	3.500E-01	60	D066	0 0 0 0 0	
1.218E-03	3.499E-01	60.05	T015	1 2 0 1 2	
1.543E-03	4.430E-01	65	D065	1 2 2 1 2	
1.542E-03	4.428E-01	65.05	T015	1 2 0 1 2	
1.849E-03	5.310E-01	69.5	D065	1 2 2 1 2	
1.848E-03	5.307E-01	69.5	T015	1 2 0 1 2	
3.315E-03	9.520E-01	84.2	D065	1 2 2 1 2	
3.312E-03	9.511E-01	84.2	T015	1 2 0 1 2	
5.638E-03	1.619E+00	96.7	D065	1 2 2 1 2	
5.629E-03	1.616E+00	96.7	T015	1 2 0 1 2	
6.112E-03	1.755E+00	98.5	D065	1 2 2 1 2	
6.101E-03	1.752E+00	98.55	T015	1 2 0 1 2	
6.129E-03	1.760E+00	99	F300	1 0 0 0 2	

1070. C_7H_6ClF
2-Fluorobenzyl chloride
o-Fluorobenzyl chloride
RN: 345-35-7 **MP** (°C)**:**
MW: 144.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.880E-03	4.164E-01	25	M342	1 0 1 1 2	
2.877E-03	4.160E-01	ns	S460	0 0 0 0 0	

1071. C_7H_6ClF
3-Fluorobenzyl chloride
m-Fluorobenzyl chloride
RN: 456-42-8 **MP** (°C)**:**
MW: 144.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-03	4.135E-01	25	M342	1 0 1 1 2	
2.858E-03	4.131E-01	ns	S460	0 0 0 0 0	

1072. C_7H_6ClF
4-Fluorobenzyl chloride
1-(Chloromethyl)-4-fluoro-benzene
α-Chloro-*p*-fluorotoluene
RN: 352-11-4 **MP** (°C)**:** –18
MW: 144.58 **BP** (°C)**:** 181.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.884E-03	4.170E-01	ns	S460	0 0 0 0 0	

1073. $C_7H_6ClN_3O_4S_2$
Chlorothiazide
Diuresal
RN: 58-94-6 **MP** (°C)**:** 342
MW: 295.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-04	2.827E-01	25	A076	1 0 1 1 2	
9.000E-04	2.662E-01	30	A089	2 0 1 1 0	EFG
9.000E-04	2.662E-01	30	A093	2 0 1 1 0	EFG
6.763E-04	2.000E-01	ns	C114	0 0 0 0 0	
7.439E-04	2.200E-01	rt	A095	0 0 2 2 1	
9.806E-04	2.900E-01	rt	B181	0 0 1 1 2	

1074. $C_7H_6ClN_4O_5S_2$
4-Nitroso-hydrochlorothiazide
RN: **MP** (°C)**:** 155–156
MW: 325.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.368E-04	2.400E-01	25	G051	1 0 1 1 0	

1075. $C_7H_6Cl_2N_2O$
Chlorambenamide
3,5-Dichloroanthranilamide
Benzamide, 2-amino-3,5-dichloro-
RN: 36765-01-2 **MP** (°C)**:** 162.5
MW: 205.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.291E-03	1.700E+00	rt	M161	0 0 0 0 1	

1076. $C_7H_6Cl_2O$
2,6-Dichloroanisole
Benzene, 1,3-dichloro-2-methoxy-
RN: 1984-65-2 **MP** (°C)**:** 31
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.908E-04	1.400E-01	25	L348	1 2 2 1 2	

1077. $C_7H_6Cl_2O$
2,3-Dichloroanisole
1,2-Dichloro-3-methoxybenzene
RN: 1984-59-4 **MP** (°C)**:** 32
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.909E-04	8.690E-02	25	L348	1 2 2 1 2	

1078. $C_7H_6Cl_2O$
2,6-Dichloro-4-methyl-phenol
2,4-Dichloro-6-methyl-phenol-
RN: 2432-12-4 **MP** (°C)**:**
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	2.833E-01	25	B316	0 0 0 0 0	
3.800E-03	6.727E-01	25	B316	0 0 0 0 0	

1079. $C_7H_6N_2O_2S$
p-Cyanobenzenesulfonamide
4-Cyanobenzenesulfonamide
RN: 3119-02-6 **MP** (°C)**:**
MW: 182.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-03	1.111E+00	15	K024	1 2 1 1 2	

1080. $C_7H_6N_2O_4$
2,4-Dinitrotoluene
2,4-Dinitro-toluol
RN: 121-14-2 **MP** (°C)**:** 71
MW: 182.14 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-03	2.709E-01	20	T301	1 2 2 2 2	
1.482E-03	2.699E-01	22	D070	1 2 0 0 1	
1.482E-03	2.700E-01	22	F300	1 0 0 0 1	
1.482E-03	2.699E-01	22	L053	1 1 0 0 1	
2.031E-03	3.699E-01	50	D070	1 2 0 0 1	
2.031E-03	3.699E-01	50	L053	1 1 0 0 1	
1.391E-02	2.534E+00	100	D070	1 2 0 0 2	
1.449E-02	2.640E+00	100	F300	1 0 0 0 2	
1.391E-02	2.534E+00	100	L053	1 1 0 0 2	

1081. $C_7H_6N_2O_5$
2,4-Dinitroanisole
Dinitroanisole
Benzene, 1-methoxy-2,4-dinitro-
RN: 119-27-7 **MP** (°C)**:** 88
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.822E-04	1.550E-01	15	D079	1 2 0 0 2	
6.863E-04	1.360E-01	50	D079	1 2 0 0 2	
2.401E-02	4.757E+00	100	D079	1 2 0 0 2	

1082. $C_7H_6N_2O_5$
Dinitrocresol
DNOC
2,4-Dinitro-6-methylphenol
Dinitro-*o*-cresol
RN: 534-52-1 **MP** (°C)**:** 86
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.561E-04	1.300E-01	15	M161	1 0 0 0 2	
6.309E-04	1.250E-01	ns	B185	0 0 0 0 0	
6.459E-04	1.280E-01	ns	M061	0 0 0 0 2	
1.000E-03	1.981E-01	ns	M163	0 0 0 0 0	EFG
1.262E-03	2.500E-01	ns	N013	0 0 0 0 2	

1083. $C_7H_6N_2S$
4-Thiocyanoaniline
Rhodan
RN: 2987-46-4 **MP** (°C)**:** 142
MW: 150.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	2.000E-01	ns	M061	0 0 0 0 0	

1084. $C_7H_6N_4$
4-Methylpteridine
Pteridine, 4-methyl-
RN: 2432-21-5 **MP** (°C)**:** 151
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.258E-01	4.762E+01	20	A083	1 2 0 0 0	

1085. $C_7H_6N_4$
7-Methylpteridine
Pteridine, 7-methyl-
RN: 936-40-3 **MP** (°C)**:** 196.5
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.775E-01	1.429E+02	20	A083	1 2 0 0 0	

1086. $C_7H_6N_4$
2-Methylpteridine
Pteridine, 2-methyl-
RN: 2432-20-4 **MP** (°C)**:** 140
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-01	1.000E+02	20	A083	1 2 0 0 0	

1087. $C_7H_6N_4O$
2-Methoxypteridine
Pteridine, 2-methoxy-
RN: 102170-44-5 **MP** (°C)**:** 150
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
1.233E+00	2.000E+02	100	A019	1 2 1 1 0	

1088. $C_7H_6N_4O$
4-Hydroxy-6-methylpteridine
4-Pteridinol, 6-methyl-
RN: 16041-24-0 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-02	3.623E+00	20	A019	2 2 1 1 2	
1.341E-01	2.174E+01	100	A019	1 2 1 1 1	

1089. $C_7H_6N_4O$
4-Hydroxy-7-methylpteridine
4-Pteridinol, 7-methyl-
RN: 34244-80-9 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.729E-02	4.425E+00	20	A019	2 2 1 1 2	
1.713E-01	2.778E+01	100	A019	1 2 1 1 1	

1090. $C_7H_6N_4O$
4-Methoxypteridine
Pteridine, 4-methoxy-
RN: 30564-38-6 **MP** (°C)**:** 195
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1091. $C_7H_6N_4O$
7-Methoxypteridine
Pteridine, 7-methoxy-
RN: 204443-27-6 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-01	1.961E+01	20	A083	1 2 0 0 0	
1.233E+00	2.000E+02	100	A083	1 2 0 0 0	

1092. $C_7H_6N_4O$
3,4-Dihydro-4-keto-3-methylpteridine
3:4-Dihydro-4-keto-3-methylpteridine
RN: 24851-65-8 **MP** (°C)**:** 286
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.686E-02	1.408E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1093. $C_7H_6N_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-acetyl-1,5-dihydro-
RN: 96448-60-1 **MP** (°C)**:**
MW: 178.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.210E-03	7.500E-01	22	B428	1 2 1 2 1	

1094. $C_7H_6N_4S$
7-Methylthiopteridine
Pteridine, 7-(methylthio)-
Pteridine-7-methyl-thiol
RN: 204443-30-1 **MP** (°C)**:**
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.792E-02	4.975E+00	20	A083	1 2 0 0 0	
1.439E-01	2.564E+01	100	A083	1 2 0 0 0	

1095. $C_7H_6N_4S$
4-Methylthiopteridine
Pteridine, 4-(methylthio)-
Pteridine-4-methyl-thiol
RN: 6966-78-5 **MP** (°C)**:** 191
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.313E-03	7.686E-01	20	A083	1 2 0 0 0	
3.100E-02	5.525E+00	100	A083	1 2 0 0 0	

1096. $C_7H_6N_4S$
4-Mercapto-7-methylpteridine
4-Pteridinethiol, 7-methyl-
RN: 98550-33-5 **MP** (°C)**:**
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.738E-03	6.662E-01	100	A083	1 2 0 0 0	

1097. $C_7H_6N_4S$
2-Methylthiopteridine
Pteridine, 2-(methylthio)-
Pteridine-2-methyl-thiol
RN: 16878-77-6 **MP** (°C)**:** 136
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.748E-02	3.115E+00	20	A083	1 2 0 0 0	
1.369E-01	2.439E+01	100	A083	1 2 0 0 0	

1098. C_7H_6O
Benzaldehyde
Benzaldehyd
RN: 100-52-7 **MP** (°C)**:** –55
MW: 106.13 **BP** (°C)**:** 179

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.251E-02	3.450E+00	20	C008	1 2 2 0 2	
2.827E-02	3.000E+00	20	F300	1 0 0 0 0	
3.754E-02	3.984E+00	25	B019	1 0 1 2 0	
3.754E-02	3.984E+00	25	B092	2 1 1 1 1	
6.549E-02	6.950E+00	25	C005	2 2 2 2 2	average
3.289E-02	3.490E+00	25	C008	1 2 2 0 2	
6.170E-02	6.548E+00	25	M017	1 2 0 1 2	
3.741E-02	3.970E+00	30	C008	1 2 2 0 2	
2.110E-02	2.239E+00	37	E028	1 0 1 1 2	
8.960E-02	9.509E+00	60	B092	2 0 1 1 1	

1099. $C_7H_6O_2$
Benzoic acid
Benzenecarboxylic acid
Benzoesaeure
RN: 65-85-0 **MP** (°C)**:** 122
MW: 122.12 **BP** (°C)**:** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-02	1.697E+00	0	F302	1 0 0 0 2	
1.390E-02	1.697E+00	0	M043	1 0 0 0 1	
1.720E-02	2.100E+00	10	F300	1 0 0 0 1	
1.716E-02	2.096E+00	10	F302	1 0 0 0 2	
1.634E-02	1.996E+00	10	M043	1 0 0 0 1	
2.010E-02	2.455E+00	15	P329	0 0 0 0 0	
1.982E-02	2.421E+00	15.5	K062	2 0 1 1 2	
2.200E-02	2.687E+00	17	B109	1 0 0 0 2	unit assumed, *sic*
2.237E-02	2.732E+00	17.7	K062	2 0 1 1 2	
2.260E-02	2.760E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
2.211E-02	2.700E+00	18	F071	1 1 2 1 2	
2.100E-02	2.565E+00	18	H009	2 1 2 2 0	EFG, 0.01N HCl
2.211E-02	2.700E+00	18	H080	1 0 0 0 2	
2.257E-02	2.756E+00	18	L050	2 0 1 2 2	
2.211E-02	2.700E+00	18	M344	1 0 0 0 2	
2.308E-02	2.819E+00	19.0	K062	2 0 1 1 2	average of 2
2.368E-02	2.892E+00	20	D041	1 0 0 0 1	
2.339E-02	2.857E+00	20	F069	2 2 2 2 2	
2.375E-02	2.900E+00	20	F300	1 0 0 0 1	
2.368E-02	2.892E+00	20	F302	1 0 0 0 2	
2.200E-02	2.686E+00	20	M038	2 2 1 1 2	
2.368E-02	2.892E+00	20	M043	1 0 0 0 1	
2.457E-02	3.000E+00	20	M049	1 0 0 0 1	
2.400E-02	2.931E+00	20	P329	0 0 0 0 0	
2.825E-02	3.450E+00	20	W026	1 0 1 1 1	average of 2
2.540E-02	3.102E+00	22	E045	2 0 1 1 2	
2.605E-02	3.181E+00	23	E045	2 0 1 1 2	
2.807E-02	3.428E+00	24.6	W029	1 2 1 1 2	
2.620E-02	3.200E+00	25	A412	1 0 2 2 1	int
2.449E-02	2.991E+00	25	B019	1 0 1 2 0	
2.751E-02	3.359E+00	25	B085	2 1 1 1 2	
2.683E-02	3.277E+00	25	B097	2 2 1 1 2	0.01M sodium benzoate
2.800E-02	3.420E+00	25	B128	1 0 1 1 2	
2.768E-02	3.381E+00	25	B302	1 0 0 0 0	pH 2.0
2.805E-02	3.426E+00	25	D058	1 0 1 1 2	
2.746E-02	3.354E+00	25	E045	2 0 1 1 2	
2.810E-02	3.432E+00	25	F001	1 0 1 2 2	
2.784E-02	3.400E+00	25	F300	1 0 0 0 1	
2.800E-02	3.419E+00	25	H009	2 1 2 2 0	EFG, 0.01N HCl
2.784E-02	3.400E+00	25	H015	1 0 0 0 1	
2.251E-03	2.749E-01	25	H060	2 0 2 0 2	*sic*
2.760E-02	3.371E+00	25	H071	2 2 2 1 2	
2.800E-02	3.419E+00	25	H084	1 0 0 0 1	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.371E+00	25	K005	1 0 0 1 2	
2.727E-02	3.330E+00	25	K047	1 2 1 2 2	
2.760E-02	3.371E+00	25	K057	2 2 1 1 2	
2.775E-02	3.389E+00	25	K064	2 2 2 1 2	
2.781E-02	3.396E+00	25	L048	1 2 2 1 2	
2.780E-02	3.395E+00	25	L050	2 0 1 2 2	
2.596E-02	3.170E+00	25	L338	1 0 1 1 2	
2.619E-02	3.199E+00	25	M038	2 2 1 1 2	
2.702E-02	3.300E+00	25	M049	1 0 0 0 1	
2.790E-02	3.407E+00	25	M116	2 1 1 1 2	
2.160E-02	2.638E+00	25	M149	2 0 2 2 2	intrinsic
2.900E-02	3.542E+00	25	O007	1 0 2 1 2	
2.268E-02	2.770E+00	25	P037	2 0 1 1 2	
2.807E-02	3.428E+00	25	P314	0 0 0 0 0	
8.820E+00	1.077E+03	25	P329	0 0 0 0 0	
2.793E-02	3.411E+00	25	R016	0 0 0 0 0	
2.781E-02	3.396E+00	25.0	K062	2 0 1 1 2	average of 2
2.700E-02	3.297E+00	25.00	M135	1 2 1 1 2	0.01N sodium benzoate
2.781E-02	3.396E+00	25.2	C096	1 0 0 1 2	
2.833E-02	3.460E+00	26	E045	2 0 1 1 2	
2.890E-02	3.529E+00	26.4	P043	2 0 1 1 2	
3.439E-02	4.200E+00	26.70	L095	2 2 1 1 2	
2.936E-02	3.586E+00	27	E045	2 0 1 1 2	
3.146E-02	3.842E+00	28	D050	1 2 1 2 2	
3.147E-02	3.843E+00	30	B109	1 0 0 0 2	unit assumed, *sic*
3.204E-02	3.913E+00	30	B109	1 0 0 0 2	unit assumed, *sic*
3.306E-02	4.037E+00	30	B118	1 0 0 0 2	
3.000E-02	3.664E+00	30	B142	2 0 1 1 0	EFG, 0.1N H_2SO_4
3.000E-02	3.664E+00	30	C077	0 0 0 0 0	
3.319E-02	4.054E+00	30	D033	2 2 1 2 2	
3.302E-02	4.033E+00	30	D061	1 0 0 0 2	
2.915E-02	3.560E+00	30	F005	1 2 2 2 2	
3.425E-02	4.182E+00	30	F302	1 0 0 0 2	
3.110E-02	3.799E+00	30	M038	2 2 1 1 2	
3.262E-02	3.984E+00	30	M043	1 0 0 0 1	
3.302E-02	4.033E+00	30	S204	2 0 1 0 2	
3.439E-02	4.200E+00	30	W026	1 0 1 1 1	average of 2
3.216E-02	3.927E+00	30.0	K062	2 0 1 1 2	average of 2
3.400E-02	4.152E+00	31	H009	2 1 2 2 0	EFG, 0.01N HCl
3.873E-02	4.730E+00	35	G052	2 1 1 1 2	
3.711E-02	4.532E+00	35	M038	2 2 1 1 2	
4.010E-02	4.897E+00	35	O007	1 0 2 1 2	
3.772E-02	4.607E+00	35	S204	2 0 1 0 2	
3.960E-02	4.836E+00	35.0	K062	2 0 1 1 2	
3.800E-02	4.641E+00	35.00	M135	1 2 1 1 2	0.01N sodium benzoate
4.201E-02	5.131E+00	37	B171	2 0 1 1 2	
3.611E-02	4.410E+00	37	F005	1 2 2 2 2	
4.200E-02	5.129E+00	37	H009	2 1 2 2 0	EFG, 0.01N HCl
3.734E-02	4.560E+00	37	M360	1 2 1 1 2	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.528E-02	5.529E+00	40	D033	2 2 1 2 2	
4.884E-02	5.964E+00	40	F302	1 0 0 0 1	
4.376E-02	5.345E+00	40	M038	2 2 1 1 2	
4.560E-02	5.569E+00	40	M043	1 0 0 0 1	
4.424E-02	5.403E+00	40	S204	2 0 1 0 2	
5.110E-02	6.241E+00	42.4	W029	1 2 1 1 2	
4.774E-02	5.830E+00	45	F005	1 2 2 2 2	
5.000E-02	6.106E+00	45	H009	2 1 2 2 0	EFG, 0.01N HCl
5.282E-02	6.451E+00	45	M038	2 2 1 1 2	
5.254E-02	6.417E+00	45	S204	2 0 1 0 2	
5.324E-02	6.502E+00	45.0	K062	2 0 1 1 2	
5.500E-02	6.717E+00	45.00	M135	1 2 1 1 2	0.01N sodium benzoate
5.463E-02	6.672E+00	45.3	S124	1 0 0 1 1	
6.878E-02	8.400E+00	50	F300	1 0 0 0 1	
6.901E-02	8.428E+00	50	F302	1 0 0 0 2	
2.107E-02	2.573E+00	50	L006	1 0 0 0 2	
6.237E-02	7.617E+00	50	S204	2 0 1 0 2	
8.032E-02	9.809E+00	53.8	S124	1 0 0 1 2	
7.048E-02	8.607E+00	55	S204	2 0 1 0 2	
8.300E-02	1.014E+01	55.40	M135	1 2 1 1 2	0.01N sodium benzoate
8.853E-02	1.081E+01	57.8	W029	1 2 1 1 2	
9.710E-02	1.186E+01	60	F302	1 0 0 0 2	
9.550E-02	1.166E+01	60	L047	1 1 2 1 2	
9.390E-02	1.147E+01	60	M043	1 0 0 0 2	
1.000E-01	1.221E+01	60.20	M135	1 2 1 1 2	0.01N sodium benzoate
1.129E-01	1.378E+01	62.5	S124	1 0 0 1 2	
1.190E-01	1.453E+01	64.60	M135	1 2 1 1 2	0.01N sodium benzoate
1.390E-01	1.698E+01	68.50	M135	1 2 1 1 2	0.01N sodium benzoate
1.527E-01	1.864E+01	69.4	S124	1 0 0 1 2	
1.424E-01	1.739E+01	70	F302	1 0 0 0 2	
1.658E-01	2.025E+01	74.1	W029	1 2 1 1 2	
1.870E-01	2.284E+01	75.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.242E-01	2.739E+01	79.0	S124	1 0 0 1 2	
2.210E-01	2.699E+01	79.30	M135	1 2 1 1 2	0.01N sodium benzoate
2.192E-01	2.676E+01	80	F302	1 0 0 0 2	
2.168E-01	2.648E+01	80	M043	1 0 0 0 2	
2.540E-01	3.102E+01	82.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.567E-01	3.135E+01	82.3	S124	1 0 0 1 2	
2.485E-01	3.035E+01	83.1	W029	1 2 1 1 2	
3.124E-01	3.815E+01	88.3	W029	1 2 1 1 2	
4.211E-01	5.142E+01	88.6	S124	1 0 0 1 2	
3.550E-01	4.335E+01	88.60	M135	1 2 1 1 2	0.01N sodium benzoate
3.564E-01	4.352E+01	90	F302	1 0 0 0 2	
4.342E-01	5.302E+01	91.5	W029	1 2 1 1 2	average of 3
5.214E-01	6.367E+01	95	D041	1 0 0 0 1	
5.208E-01	6.360E+01	95	F300	1 0 0 0 2	
5.214E-01	6.367E+01	95	F302	1 0 0 0 2	
4.977E-01	6.078E+01	95.3	W029	1 2 1 1 2	
5.493E-01	6.708E+01	98.6	W029	1 2 1 1 2	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.547E-01	5.553E+01	100	M043	1 0 0 0 2	
8.241E-01	1.006E+02	109.4	W029	1 2 1 1 2	
1.399E+00	1.709E+02	116.1	W029	1 2 1 1 2	
2.594E+00	3.168E+02	116.3	W029	1 2 1 1 2	
2.001E+00	2.444E+02	117.2	W029	1 2 1 1 2	
9.000E-04	1.099E-01	ns	D037	1 1 1 1 0	pH 3.0, intrinsic

1100. $C_7H_6O_2$

m-Hydroxybenzaldehyde
3-Hydroxy-benzaldehyd

RN: 100-83-4 **MP** (°C)**:** 104
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.252E-01	2.750E+01	43	F300	1 0 0 0 2	

1101. $C_7H_6O_2$

p-Hydroxybenzaldehyde
4-Hydroxy-benzaldehyd

RN: 123-08-0 **MP** (°C)**:** 213.5
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-01	1.290E+01	30	F300	1 0 0 0 2	

1102. $C_7H_6O_2$

Salicylaldehyde
Salicylaldehyd

RN: 90-02-8 **MP** (°C)**:** –7
MW: 122.12 **BP** (°C)**:** 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-04	8.077E-02	25	K129	2 1 2 2 2	
1.392E-01	1.700E+01	86	F300	1 0 0 0 1	

1103. $C_7H_6O_3$

Salicylic acid
2-Hydroxybenzoic acid
o-Hydroxybenzoic acid

RN: 69-72-7 **MP** (°C)**:** 158
MW: 138.12 **BP** (°C)**:** 211

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.799E-03	9.391E-01	0	C083	1 2 1 1 2	
5.792E-03	8.000E-01	0	F300	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 1	
9.472E-03	1.308E+00	10	B074	1 2 1 2 2	
8.688E-03	1.200E+00	10	F300	1 0 0 0 1	
1.084E-02	1.498E+00	10	M043	1 0 0 0 0	
1.084E-02	1.498E+00	10	M043	1 0 0 0 1	
8.656E-03	1.196E+00	10	N420	0 0 0 0 0	
9.327E-03	1.288E+00	10	W044	1 0 1 0 2	
1.108E-02	1.531E+00	9.99	A341	0 0 0 0 0	
1.009E-02	1.393E+00	12.1	W044	1 0 1 0 2	
1.207E-02	1.667E+00	14.5	D061	1 0 0 0 2	
1.209E-02	1.670E+00	14.50	B118	1 0 0 0 2	unit assumed
1.028E-02	1.420E+00	15	H022	1 2 2 2 2	
1.520E-03	2.100E-01	15	M461	0 0 0 0 0	
9.875E-03	1.364E+00	15	N420	0 0 0 0 0	
1.258E-02	1.737E+00	17	K046	1 0 0 0 2	spray-dried product
1.330E-02	1.837E+00	20	B074	1 2 1 2 2	
1.303E-02	1.800E+00	20	F071	1 1 2 1 2	
1.303E-02	1.800E+00	20	F300	1 0 0 0 1	
1.303E-02	1.800E+00	20	H080	1 0 0 0 2	
1.296E-02	1.790E+00	20	K047	1 2 1 2 2	
1.445E-02	1.996E+00	20	M043	1 0 0 0 1	
1.445E-02	1.996E+00	20	M043	1 0 0 0 0	
1.445E-02	1.996E+00	20	M107	2 2 1 1 0	EFG
1.303E-02	1.800E+00	20	M344	1 0 0 0 2	
1.154E-02	1.594E+00	20	N420	0 0 0 0 0	
1.593E-02	2.200E+00	20	W026	1 0 1 1 1	average of 2
1.330E-02	1.837E+00	20	W044	1 0 1 0 2	
1.520E-02	2.100E+00	21	B331	1 2 2 1 0	pH 7.4
1.390E-02	1.920E+00	22	E045	2 0 1 1 2	
1.470E-02	2.030E+00	23	E045	2 0 1 1 2	
1.474E-02	2.036E+00	23.0	W044	1 0 1 0 2	
1.550E-02	2.141E+00	24	E045	2 0 1 1 2	
1.847E-02	2.551E+00	24.99	A341	0 0 0 0 0	
1.590E-02	2.196E+00	25	B090	1 1 1 1 2	
1.633E-02	2.255E+00	25	C083	1 2 1 1 2	
1.630E-02	2.251E+00	25	E045	2 0 1 1 2	
1.593E-02	2.200E+00	25	H007	0 0 0 0 0	
1.620E-02	2.238E+00	25	H084	1 0 0 0 2	
1.084E-02	1.498E+00	25	H129	1 0 0 1 0	

(*continued*)

1103. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	2.228E+00	25	K040	1 0 2 1 2	
1.634E-02	2.257E+00	25	K053	2 2 2 2 2	
1.620E-02	2.238E+00	25	K057	2 2 1 1 2	
1.601E-02	2.211E+00	25	L050	2 0 1 2 2	
1.665E-03	2.300E-01	25	M461	0 0 0 0 0	
1.370E-02	1.892E+00	25	N420	0 0 0 0 0	
1.680E-02	2.320E+00	25	O007	1 0 2 1 2	
1.621E-02	2.239E+00	25	P314	0 0 0 0 0	
1.491E-02	2.059E+00	25.50	A012	2 2 2 2 2	
1.700E-02	2.348E+00	26	E045	2 0 1 1 2	
1.780E-02	2.459E+00	27	E045	2 0 1 1 2	
1.746E-02	2.411E+00	27	K046	1 0 0 0 2	spray-dried product
1.728E-02	2.387E+00	28	D050	1 2 1 2 2	
1.784E-02	2.464E+00	28.1	W044	1 0 1 0 2	
1.360E-02	1.878E+00	30	A065	2 0 2 2 1	
1.885E-02	2.603E+00	30	B074	1 2 1 2 2	
1.987E-02	2.745E+00	30	B118	1 0 0 0 2	unit assumed
1.750E-02	2.417E+00	30	B142	2 0 1 1 0	EFG, 0.1N H_2SO_4
1.800E-02	2.486E+00	30	C077	0 0 0 0 0	
1.986E-02	2.743E+00	30	D061	1 0 0 0 2	
1.426E-02	1.970E+00	30	F005	1 2 2 2 2	
1.796E-02	2.481E+00	30	H022	1 2 2 2 2	
1.700E-02	2.348E+00	30	K020	1 0 1 1 0	EFG
1.868E-02	2.580E+00	30	K047	1 2 1 2 2	
2.022E-02	2.792E+00	30	M043	1 0 0 0 0	
2.022E-02	2.792E+00	30	M043	1 0 0 0 1	
2.165E-02	2.991E+00	30	M107	2 2 1 1 0	EFG
2.244E-03	3.100E-01	30	M461	0 0 0 0 0	
1.685E-02	2.327E+00	30	N420	0 0 0 0 0	
2.244E-02	3.100E+00	30	W026	1 0 1 1 2	average of 2
1.906E-02	2.633E+00	30	W044	1 0 1 0 2	
2.172E-02	3.000E+00	30.6	P014	2 1 2 2 0	
2.442E-02	3.373E+00	33.99	A341	0 0 0 0 0	
2.201E-02	3.041E+00	34.4	W044	1 0 1 0 2	
2.273E-02	3.140E+00	35	K047	1 2 1 2 2	
2.039E-02	2.816E+00	35	N420	0 0 0 0 0	
2.390E-02	3.301E+00	35	O007	1 0 2 1 2	
1.332E-02	1.840E+00	37	B171	2 0 1 1 2	
1.861E-02	2.570E+00	37	C079	0 0 0 0 0	
1.897E-02	2.620E+00	37	F005	1 2 2 2 2	
2.452E-02	3.386E+00	37	K046	1 0 0 0 2	spray-dried product
1.303E-02	1.800E+00	37	Y421	0 0 0 0 0	
2.590E-02	3.577E+00	38.7	W044	1 0 1 0 2	
2.848E-02	3.934E+00	40	B074	1 2 1 2 2	
2.679E-02	3.700E+00	40	F300	1 0 0 0 1	
2.672E-02	3.690E+00	40	K047	1 2 1 2 2	
3.028E-02	4.182E+00	40	M043	1 0 0 0 1	

(*continued*)

1103. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-02	4.182E+00	40	M043	1 0 0 0 0	
2.884E-02	3.984E+00	40	M107	2 2 1 1 0	EFG
4.561E-03	6.300E-01	40	M461	0 0 0 0 0	
2.502E-02	3.456E+00	40	N420	0 0 0 0 0	
2.719E-02	3.756E+00	40	W044	1 0 1 0 2	
3.167E-02	4.374E+00	43.99	A341	0 0 0 0 0	
3.743E-02	5.170E+00	44.99	A341	0 0 0 0 0	
2.462E-02	3.400E+00	45	F005	1 2 2 2 2	
3.059E-02	4.226E+00	45	N420	0 0 0 0 0	
3.714E-02	5.130E+00	46.99	A341	0 0 0 0 0	
3.562E-02	4.921E+00	47	K046	1 0 0 0 2	spray-dried product
3.681E-02	5.084E+00	48.6	W044	1 0 1 0 2	
4.102E-02	5.665E+00	49.99	A341	0 0 0 0 0	
4.261E-02	5.885E+00	50	B074	1 2 1 2 2	
6.154E-03	8.500E-01	50	M461	0 0 0 0 0	
3.769E-02	5.206E+00	50	N420	0 0 0 0 0	
3.889E-02	5.371E+00	50	W044	1 0 1 0 2	
4.337E-02	5.991E+00	50.99	A341	0 0 0 0 0	
4.677E-02	6.461E+00	51.99	A341	0 0 0 0 0	
5.151E-02	7.115E+00	53.99	A341	0 0 0 0 0	
5.319E-02	7.347E+00	54.99	A341	0 0 0 0 0	
4.947E-02	6.833E+00	56.0	W044	1 0 1 0 2	
6.104E-02	8.431E+00	57.49	A341	0 0 0 0 0	
6.202E-02	8.566E+00	60	B074	1 2 1 2 2	
6.009E-02	8.300E+00	60	F300	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 0	
5.888E-02	8.133E+00	60	W044	1 0 1 0 2	
7.184E-02	9.922E+00	61.49	A341	0 0 0 0 0	
7.140E-02	9.862E+00	64.0	W044	1 0 1 0 2	
8.184E-02	1.130E+01	65.99	A341	0 0 0 0 0	
8.373E-02	1.156E+01	66.0	W044	1 0 1 0 2	
1.252E-01	1.730E+01	75.0	W044	1 0 1 0 2	
1.499E-01	2.070E+01	80	F300	1 0 0 0 2	
1.600E-01	2.210E+01	80	M043	1 0 0 0 0	
1.600E-01	2.210E+01	80	M043	1 0 0 0 2	
5.437E-01	7.510E+01	100	M043	1 0 0 0 0	
5.437E-01	7.510E+01	100	M043	1 0 0 0 2	
1.598E-02	2.207E+00	ns	O003	0 2 1 1 2	
1.514E-02	2.091E+00	ns	R427	0 0 0 0 0	
1.841E-02	2.544E+00	rt	H431	0 0 0 0 0	

1104. $C_7H_6O_3$

Protocatechualdehyde
3,4-Dihydroxy-benzaldehyd
RN: 139-85-5 **MP** (°C)**:**
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.620E-01	5.000E+01	20	F300	1 0 0 0 0	
~1.88E+00	~2.60E+02	100	F300	1 0 0 0 0	

1105. $C_7H_6O_3$

p-Hydroxybenzoic acid
4-Hydroxy-benzoesaeure
4-Hydroxybenzoic acid
p-Hydroxybenzoicacid
4-Hydroxybenzenecarboxylic acid
RN: 99-96-7 **MP** (°C)**:** 214.5
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-02	2.494E+00	0	M043	1 0 0 0 1	
1.590E-02	2.196E+00	4.99	A405	2 0 1 1 2	
2.525E-02	3.488E+00	10	M043	1 0 0 0 1	
2.280E-02	3.149E+00	10.99	A405	2 0 1 1 2	
2.216E-02	3.061E+00	12.7	W044	1 0 1 0 2	
5.746E-02	7.937E+00	15	D041	1 0 0 0 0	
3.186E-02	4.400E+00	15	F300	1 0 0 0 1	
2.624E-02	3.624E+00	15	H022	1 2 2 2 2	
2.990E-02	4.130E+00	15.99	A405	2 0 1 1 2	
3.740E-02	5.166E+00	19.99	A405	2 0 1 1 2	
3.470E-02	4.793E+00	20	C006	1 2 1 1 2	
3.817E-02	5.272E+00	20	M043	1 0 0 0 1	
3.602E-02	4.975E+00	20	M107	2 2 1 1 0	EFG
3.545E-02	4.896E+00	20.9	W044	1 0 1 0 2	
4.890E-02	6.754E+00	24.99	A405	2 0 1 1 2	
3.545E-02	4.896E+00	25	D081	1 1 2 1 2	
6.580E-02	9.089E+00	25	D339	0 0 0 0 0	
4.634E-02	6.400E+00	25	H007	0 0 0 0 0	
3.318E-02	4.583E+00	25	M334	1 2 1 1 2	
4.322E-02	5.970E+00	25	N023	1 2 2 1 2	hydrate
6.241E-02	8.620E+00	25	N023	1 2 2 1 2	anhydrate
3.873E-02	5.350E+00	25.50	A012	2 2 2 2 2	
6.340E-02	8.757E+00	29.99	A405	2 0 1 1 2	
5.400E-02	7.459E+00	30	A065	2 0 2 2 1	
4.800E-02	6.630E+00	30	C077	0 0 0 0 0	
5.500E-02	7.597E+00	30	H019	0 0 0 0 0	
5.421E-02	7.488E+00	30	H022	1 2 2 2 2	
5.500E-02	7.597E+00	30	K020	1 0 1 1 0	EFG

(*continued*)

1105. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-02	7.937E+00	30	M043	1 0 0 0 1	
5.746E-02	7.937E+00	30	M107	2 2 1 1 0	EFG
5.538E-02	7.650E+00	30	N023	1 2 2 1 2	hydrate
7.790E-02	1.076E+01	30	N023	1 2 2 1 2	anhydrate
5.496E-02	7.592E+00	30	W044	1 0 1 0 2	
8.120E-02	1.122E+01	33.99	A405	2 0 1 1 2	
7.076E-02	9.774E+00	34.4	W044	1 0 1 0 2	
7.247E-02	1.001E+01	35	N023	1 2 2 1 2	hydrate
9.781E-02	1.351E+01	35	N023	1 2 2 1 2	anhydrate
1.231E-01	1.700E+01	37	B171	2 0 1 1 2	
1.027E-01	1.419E+01	38.99	A405	2 0 1 1 2	
8.663E-02	1.197E+01	39.4	W044	1 0 1 0 2	
8.938E-02	1.235E+01	40	M043	1 0 0 0 2	
9.996E-02	1.381E+01	40	M107	2 2 1 1 0	EFG
1.203E-01	1.662E+01	40	N023	1 2 2 1 2	anhydrate
9.339E-02	1.290E+01	40	N023	1 2 2 1 2	hydrate
1.385E-01	1.913E+01	42.99	A405	2 0 1 1 2	
1.291E-01	1.783E+01	46.0	W044	1 0 1 0 2	
1.804E-01	2.492E+01	47.99	A405	2 0 1 1 2	
2.438E-01	3.367E+01	52.99	A405	2 0 1 1 2	
1.931E-01	2.667E+01	54.6	W044	1 0 1 0 2	
3.330E-01	4.600E+01	56.99	A405	2 0 1 1 2	
2.978E-01	4.114E+01	60	M043	1 0 0 0 2	
4.286E-01	5.920E+01	61.99	A405	2 0 1 1 2	
5.666E-01	7.826E+01	66.99	A405	2 0 1 1 2	
7.269E-01	1.004E+02	71.99	A405	2 0 1 1 2	
1.835E-01	2.534E+01	75	D041	1 0 0 0 1	
8.723E-01	1.205E+02	80	M043	1 0 0 0 2	
1.875E+00	2.590E+02	100	F300	1 0 0 0 2	
2.410E+00	3.329E+02	100	M043	1 0 0 0 2	
3.715E-02	5.132E+00	ns	R427	0 0 0 0 0	
4.854E-02	6.705E+00	rt	H431	0 0 0 0 0	

1106. $C_7H_6O_3$

β-2-Furyncrylic acid
β-2-Furylacrylic acid
β-Furyl-(2)-acrylsaeure

RN: 539-47-9 **MP** (°C)**:** 143
MW: 138.12 **BP** (°C)**:** 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.448E-02	2.000E+00	20	F300	1 0 0 0 0	

1107. $C_7H_6O_3$

m-Hydroxybenzoic acid
3-Hydroxy-benzoesaeure
3-Hydroxybenzoic acid
m-Hydroxybenzoicacid

RN: 99-06-9 **MP** (°C)**:** 202
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	3.488E+00	0	M043	1 0 0 0 1	
3.960E-02	5.470E+00	10	M043	1 0 0 0 1	
4.804E-02	6.636E+00	13.3	W044	1 0 1 0 2	
5.068E-02	7.000E+00	15	F300	1 0 0 0 1	
4.477E-02	6.184E+00	15	H022	1 2 2 2 2	
6.052E-02	8.360E+00	18.8	W044	1 0 1 0 2	
6.173E-02	8.527E+00	20	M043	1 0 0 0 1	
4.318E-02	5.964E+00	20	M107	2 2 1 1 0	EFG
7.551E-02	1.043E+01	24.3	W044	1 0 1 0 2	
5.249E-02	7.250E+00	25.50	A012	2 2 2 2 2	
7.800E-03	1.077E+00	30	A065	2 0 2 2 1	
8.600E-02	1.188E+01	30	C077	0 0 0 0 0	
8.800E-02	1.215E+01	30	H019	0 0 0 0 0	
8.300E-02	1.146E+01	30	H021	1 2 1 1 0	EFG
9.291E-02	1.283E+01	30	M043	1 0 0 0 1	
6.813E-02	9.411E+00	30	M107	2 2 1 1 0	EFG
9.552E-02	1.319E+01	30	W044	1 0 1 0 2	
9.855E-02	1.361E+01	30.9	W044	1 0 1 0 2	
1.271E-01	1.756E+01	36.2	W044	1 0 1 0 2	
1.420E-01	1.961E+01	40	M043	1 0 0 0 1	
1.105E-01	1.526E+01	40	M107	2 2 1 1 0	EFG
2.809E-01	3.880E+01	50	F300	1 0 0 0 1	
2.222E-01	3.070E+01	51.0	W044	1 0 1 0 2	
3.118E-01	4.306E+01	60	M043	1 0 0 0 1	
7.987E-01	1.103E+02	80	M043	1 0 0 0 2	
2.678E+00	3.699E+02	100	M043	1 0 0 0 2	
1.810E-02	2.500E+00	ns	B361	0 0 0 0 0	
5.012E-02	6.923E+00	ns	R427	0 0 0 0 0	

1108. $C_7H_6O_4$

2,6-Dihydroxybenzoic acid
2,6-Dihydroxy-benzoesaeure
γ-Resorcylic acid

RN: 303-07-1 **MP** (°C)**:**
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-02	9.556E+00	ns	C014	0 0 0 1 1	

1109. $C_7H_6O_4$
Protocatechuic acid
3,4-Dihydroxy-benzoesaeure
3,4-Dihydroxybenzoic acid
RN: 99-50-3 **MP** (°C)**:**
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.181E-01	1.820E+01	14	F300	1 0 0 0 2	
1.440E+00	2.220E+02	80	F300	1 0 0 0 2	

1110. $C_7H_6O_4$
β-Resorcyclic acid
2,4-Dihydroxy-benzoesaeure
2,4-Dihydroxybenzoic acid
2,4-Dihydroxybenzoicacid
β-Resorcylic acid
4-Hydroxysalicylic acid
RN: 89-86-1 **MP** (°C)**:** 225
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.893E-02	6.000E+00	25	H007	0 0 0 0 0	

1111. $C_7H_6O_4$
Gentisic acid
2,5-Dihydroxy-benzoesaeure
2,5-Dihydroxybenzoic acid
2,5-Dihydroxybenzoicacid
Hydroquinonecarboxylic acid
RN: 490-79-9 **MP** (°C)**:** 205
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-01	2.200E+01	25	H007	0 0 0 0 0	

1112. $C_7H_6O_5$
Gallic acid
3,4,5-Trihydroxybenzoesaeure
Gallussaeure
RN: 149-91-7 **MP** (°C)**:** 250
MW: 170.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E+00	2.253E+02	–10.0	L430	0 0 0 0 0	
5.349E-02	9.100E+00	15	M461	0 0 0 0 0	
5.589E-02	9.509E+00	19.99	L430	0 0 0 0 0	

(*continued*)

1112. $C_7H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.995E-02	1.190E+01	20	F300	1 0 0 0 2	
5.820E-02	9.901E+00	24.99	L430	0 0 0 0 0	
8.641E-02	1.470E+01	25	M461	0 0 0 0 0	
8.001E-02	1.361E+01	29.99	L430	0 0 0 0 0	
1.093E-01	1.860E+01	30	M461	0 0 0 0 0	
1.034E-01	1.759E+01	34.99	L430	0 0 0 0 0	
1.355E-01	2.306E+01	39.99	L430	0 0 0 0 0	
1.552E-01	2.640E+01	40	M461	0 0 0 0 0	
1.751E-01	2.979E+01	44.99	L430	0 0 0 0 0	
2.272E-01	3.865E+01	49.99	L430	0 0 0 0 0	
2.240E-01	3.810E+01	50	M461	0 0 0 0 0	
2.879E-01	4.898E+01	54.99	L430	0 0 0 0 0	
3.774E-01	6.420E+01	59.99	L430	0 0 0 0 0	
4.470E-01	7.604E+01	64.99	L430	0 0 0 0 0	
6.044E-01	1.028E+02	69.99	L430	0 0 0 0 0	
7.064E-01	1.202E+02	74.99	L430	0 0 0 0 0	
9.497E-01	1.616E+02	79.99	L430	0 0 0 0 0	
1.198E+00	2.038E+02	84.99	L430	0 0 0 0 0	
1.505E+00	2.561E+02	100	F300	1 0 0 0 2	
4.202E-02	7.149E+00	–.0	L430	0 0 0 0 0	
6.918E-02	1.177E+01	ns	R427	0 0 0 0 0	

1113. $C_7H_6O_5$

2,3,4-Trihydroxybenzoic acid
2,3,4-Trihydroxybenzoesaeure

RN: 610-02-6 **MP** (°C)**:**
MW: 170.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.878E-03	1.000E+00	12.50	F300	1 0 0 0 0	

1114. C_7H_7Br

m-Bromotoluene
3-Bromotoluene
3-Methyl-1-bromobenzene
1-Bromo-3-methylbenzene
3-Bromo-1-methylbenzene
3-Methylphenyl bromide

RN: 591-17-3 **MP** (°C)**:** –39.8
MW: 171.04 **BP** (°C)**:** 183.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	5.131E-02	ns	O013	0 1 0 1 0	
3.020E-04	5.165E-02	ns	S460	0 0 0 0 0	

1115. C_7H_7Cl

m-Chlorotoluene
3-Chlorotoluene
1-Chloro-3-methylbenzene
m-Tolyl chloride

RN: 108-41-8 **MP** (°C)**:** –48
MW: 126.59 **BP** (°C)**:** 161.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1116. C_7H_7Cl

o-Chlorotoluene
2-Chlorotoluene
2-Chloro-1-methylbenzene
2-Methylchlorobenzene
1-Methyl-2-chlorobenzene
OCT

RN: 95-49-8 **MP** (°C)**:** –36
MW: 126.59 **BP** (°C)**:** 159.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1117. C_7H_7Cl

p-Chlorotoluene
4-Chlorotoluene
p-Tolyl chloride
4-Chloro-1-methyl-benzene
PCT
1-Chloro-4-methylbenzene

RN: 106-43-4 **MP** (°C)**:** 8
MW: 126.59 **BP** (°C)**:** 162.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-04	1.065E-01	20	H118	1 1 1 1 2	
1.084E-03	1.372E-01	20	H301	0 0 0 0 0	
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1118. $C_7H_7ClN_2O_4S$

Saluamine
2-Amino-4-chloro-5-sulfamoylbenzoic acid
4-Chloro-5-sulfamylanthranilic acid
Desfurylmethylfurosemide
4-Chloro-5-sulfamoylanthranilic acid
-Amino-5-aminosulfonyl-4-chlorobenzoic acid
RN: 3086-91-7 **MP** (°C)**:**
MW: 250.66 **BP** (°C)**:** 549.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.218E-03	5.560E-01	25	B405	1 1 1 2 2	Buffer pH 2.0
3.008E-03	7.540E-01	25	B405	1 1 1 2 2	

1119. $C_7H_7ClN_4O_2$

8-Chlorotheophylline
8-Chloro-1,3-dimethyl-2,6(1H,3H)-purinedione
RN: 85-18-7 **MP** (°C)**:** 290
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.481E-01	ns	R427	0 0 0 0 0	

1120. C_7H_7ClO

Chlorocresol
3-Methyl-4-chlorophenol
4-Chloro-3-cresol
6-Chloro-3-hydroxytoluene
3-Methyl-4-chloro-phenol-
Phenol, 4-chloro-3-methyl-
RN: 59-50-7 **MP** (°C)**:** 67
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	3.992E+00	25	B316	0 0 0 0 0	
3.489E-02	4.975E+00	25	R041	0 0 0 0 0	
3.647E-02	5.200E+00	ns	G024	0 0 0 0 2	

1121. C_7H_7ClO

4-Chloroanisole
p-Chloroanisole
1-Chloro-4-methoxybenzene
RN: 623-12-1 **MP** (°C)**:** –18
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.662E-03	2.370E-01	25	L348	1 2 2 1 2	

1122. C_7H_7ClO

2-Methyl-6-chloro-phenol
2-Chloro-6-methylphenol
6-Chloro-*o*-cresol
3-Chloro-2-hydroxytoluene
6-Chloro-2-methylphenol

RN: 87-64-9 **MP** (°C)**:**
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.565E+00	25	B316	0 0 0 0 0	

1123. C_7H_7ClO

2-Methyl-4-chloro-phenol
4-Chloro-*o*-cresol
4-Chloro-2-methylphenol
5-Chloro-2-hydroxytoluene

RN: 1570-64-5 **MP** (°C)**:** 45–48
MW: 142.59 **BP** (°C)**:** 220–225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-02	6.844E+00	25	B316	0 0 0 0 0	

1124. C_7H_7ClO

2-Chloroanisole
o-Chloroanisole

RN: 766-51-8 **MP** (°C)**:** –27
MW: 142.59 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.437E-03	4.900E-01	25	L348	1 2 2 1 2	
3.467E-03	4.944E-01	ns	S460	0 0 0 0 0	

1125. C_7H_7ClO

3-Chloroanisole
m-Chloroanisole
1-Chloro-3-methoxybenzene

RN: 2845-89-8 **MP** (°C)**:** <25
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-03	2.350E-01	25	L348	1 2 2 1 2	
1.660E-03	2.366E-01	ns	S460	0 0 0 0 0	

1126. $C_7H_7Cl_2NO$

Clopidol
3,5-Dichloro-2,6-dimethyl-4-pyridinol
Coyden
Methylchloropindol
RN: 2971-90-6 **MP** (°C)**:**
MW: 192.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-04	4.000E-02	ns	K138	0 0 0 0 1	

1127. $C_7H_7Cl_3NO_3PS$

Chlorpyrifos-methyl
Chlorpyrifos-methy
RN: 5598-13-0 **MP** (°C)**:**
MW: 322.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
9.922E-06	3.200E-03	20	B300	2 1 1 1 2	
9.922E-06	3.200E-03	20	B324	0 0 0 0 0	
9.921E-06	3.200E-03	20	B324	0 0 0 0 0	
1.476E-05	4.760E-03	20	C053	0 0 0 0 0	
1.240E-05	4.000E-03	24	K069	2 0 0 1 1	
1.240E-05	4.000E-03	25	M161	1 0 0 0 0	
2.139E-05	6.899E-03	30	B324	0 0 0 0 0	
2.139E-05	6.900E-03	30	B324	0 0 0 0 0	
1.476E-05	4.760E-03	ns	F071	0 1 2 1 2	
1.240E-05	4.000E-03	ns	K138	0 0 0 0 1	
1.643E-05	5.300E-03	ns	M110	0 0 0 0 0	EFG

1128. $C_7H_7Cl_3NO_4P$

Torelle
Dimethyl 3,5,6-trichloro-2-pyridinyl phosphate
DOWCO 217
Fospirate
Phosphoric acid, dimethyl 3,5,6-trichloro-2-pyridyl ester
RN: 5598-52-7 **MP** (°C)**:**
MW: 306.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.789E-04	3.000E-01	24	K069	2 0 0 1 1	

1129. $C_7H_7FN_2O_3$
3-Propionyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Propionyl-5-fluorouracil
RN: 75410-16-1 **MP** (°C)**:** 113–114
MW: 186.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-01	3.530E+01	22	B321	0 0 0 0 0	pH 4.0
1.896E-01	3.530E+01	22	B332	1 1 0 0 1	pH 4.0
1.980E-01	3.686E+01	22	B416	2 2 1 2 1	

1130. $C_7H_7FN_2O_4$
3-Acetoxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Acetoxymethyl-5-fluorouracil
RN: 73042-04-3 **MP** (°C)**:** 158–159
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.894E-02	2.000E+01	22	B321	0 0 0 0 0	pH 4.0

1131. $C_7H_7FN_2O_4$
1-Acetoxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Acetoxymethyl-5-fluorouracil
RN: 62113-41-1 **MP** (°C)**:** 122–123
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.132E-01	4.310E+01	22	B321	0 0 0 0 0	pH 4.0

1132. $C_7H_7FN_2O_4$
3-Ethyloxycarbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Ethyloxycarbonyl-5-fluorouracil
1-Ethyloxycarbonyl-5-fluorouracil
RN: 75410-27-4 **MP** (°C)**:** 126–128
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E-01	7.200E+01	22	B321	0 0 0 0 0	pH 4.0
3.413E-02	6.900E+00	22	B332	1 1 0 0 1	pH 4.0

1133. C_7H_7NO

Benzamide
Benzamid
Phenyl carboxamide
Benzoic acid amide

RN: 55-21-0 **MP** (°C)**:** 130
MW: 121.14 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.923E-02	5.964E+00	10	M043	1 0 0 0 0	
4.750E-02	5.754E+00	12	O019	1 0 0 1 2	
1.000E-01	1.211E+01	20	B139	2 1 1 1 1	
8.173E-02	9.901E+00	20	M043	1 0 0 0 1	
1.100E-01	1.333E+01	22	J037	0 0 0 0 0	
1.106E-01	1.340E+01	25	F300	1 0 0 0 2	
1.059E-01	1.283E+01	30	M043	1 0 0 0 1	
1.300E-01	1.575E+01	40	M043	1 0 0 0 1	
1.651E-01	2.000E+01	50	P064	2 0 1 1 1	
3.931E-01	4.762E+01	60	M043	1 0 0 0 0	
6.191E-01	7.500E+01	70	P064	2 0 1 1 1	
5.503E+00	6.667E+02	80	M043	1 0 0 0 2	
6.686E+00	8.100E+02	90	P064	2 0 1 1 2	
7.338E+00	8.889E+02	100	M043	1 0 0 0 2	
7.842E+00	9.500E+02	110	P064	2 0 1 1 2	
1.100E-01	1.332E+01	rt	D021	0 0 1 1 2	

1134. $C_7H_7NO_2$

Salicylamide
2-Hydroxybenzoicacidamide
Algamon
Amid-sal
Amidosal
Algiamida

RN: 65-45-2 **MP** (°C)**:** 140
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.878E-03	1.218E+00	10	N419	0 0 0 0 0	
1.060E-02	1.454E+00	15	D012	1 1 0 1 2	
1.137E-02	1.559E+00	15	N419	0 0 0 0 0	
1.100E-02	1.509E+00	16	D012	1 1 0 1 2	
1.531E-02	2.100E+00	20	E046	1 0 0 0 0	EFG
1.447E-02	1.985E+00	20	N419	0 0 0 0 0	
1.900E-02	2.606E+00	22	J031	0 0 0 0 0	
1.604E-02	2.200E+00	23	B328	1 2 2 1 1	pH 4.0
1.500E-02	2.057E+00	25	D012	1 1 0 1 2	
1.750E-02	2.400E+00	25	E046	1 0 0 0 0	EFG
1.757E-02	2.409E+00	25	N419	0 0 0 0 0	
1.831E-02	2.511E+00	25	P314	0 0 0 0 0	

(*continued*)

1134. $C_7H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.115E-02	2.900E+00	30	E046	1 0 0 0 0	EFG
2.166E-02	2.970E+00	30	N419	0 0 0 0 0	
2.771E-02	3.800E+00	35	E046	1 0 0 0 0	EFG
2.685E-02	3.682E+00	35	N419	0 0 0 0 0	
2.900E-02	3.977E+00	37	D012	1 1 0 1 2	
3.427E-02	4.700E+00	40	E046	1 0 0 0 0	EFG
3.285E-02	4.505E+00	40	N419	0 0 0 0 0	
4.280E-02	5.870E+00	45	D012	1 1 0 1 2	
4.181E-02	5.734E+00	45	N419	0 0 0 0 0	
5.323E-02	7.300E+00	50	E046	1 0 0 0 0	EFG
5.371E-02	7.366E+00	50	N419	0 0 0 0 0	
1.677E-03	2.300E-01	ns	B361	0 0 0 0 0	

1135. $C_7H_7NO_2$

p-Aminobenzoic acid
4-Amino-benzoesaeure
4-Aminobenzoic acid
p-Aminobenzoicacid
1-Amino-4-carboxybenzene

RN: 150-13-0 **MP** (°C)**:** 187.0
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.479E-02	3.400E+00	12.80	F300	1 0 0 0 1	
3.609E-02	4.950E+00	18	C033	1 0 2 1 2	
3.628E-02	4.975E+00	25	D041	1 0 0 0 0	
3.930E-02	5.390E+00	25	L338	1 0 1 1 2	
3.646E-02	5.000E+00	25	M054	1 0 0 0 0	
3.500E-02	4.800E+00	25	P015	0 0 0 0 0	
4.455E-02	6.110E+00	30	C033	1 0 2 1 2	
4.579E-02	6.280E+00	30	H018	0 0 0 0 0	
4.500E-02	6.171E+00	30	L069	1 0 1 1 0	EFG
6.125E-02	8.400E+00	37	B171	2 0 1 1 2	
6.040E-02	8.283E+00	37	F006	1 1 2 2 2	

1136. $C_7H_7NO_2$

o-Nitrotoluene
2-Nitro-toluol
2-Nitrotoluene

RN: 88-72-2 **MP** (°C)**:** –9.5
MW: 137.14 **BP** (°C)**:** 221.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.872E-03	5.310E-01	9.99	B403	1 2 2 2 2	
4.441E-03	6.090E-01	19.99	B403	1 2 2 2 2	

(*continued*)

1136. $C_7H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.017E-03	6.880E-01	29.99	B403	1 2 2 2 2	
4.740E-03	6.500E-01	30	F300	1 0 0 0 2	
5.637E-03	7.730E-01	39.99	B403	1 2 2 2 2	

1137. $C_7H_7NO_2$

o-Aminobenzoic acid
2-Aminobenzoic acid
Anthranilsaeure

RN: 118-92-3 **MP** (°C)**:** 145
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.181E-02	2.991E+00	10	M043	1 0 0 0 0	
2.543E-02	3.488E+00	14	D041	1 0 0 0 1	
2.552E-02	3.500E+00	14	F300	1 0 0 0 1	
2.543E-02	3.488E+00	20	M043	1 0 0 0 1	
4.349E-02	5.964E+00	30	M043	1 0 0 0 0	
6.504E-02	8.920E+00	40	M043	1 0 0 0 0	
3.552E+00	4.872E+02	100	M043	1 0 0 0 1	

1138. $C_7H_7NO_2$

m-Nitrotoluene
3-Nitro-toluol
3-Nitrotoluene

RN: 99-08-1 **MP** (°C)**:** 16
MW: 137.14 **BP** (°C)**:** 232.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.281E-03	4.500E-01	9.99	B403	1 2 2 2 2	
3.580E-03	4.910E-01	19.99	B403	1 2 2 2 2	
3.894E-03	5.340E-01	29.99	B403	1 2 2 2 2	
3.646E-03	5.000E-01	30	F300	1 0 0 0 2	
4.120E-03	5.650E-01	39.99	B403	1 2 2 2 2	

1139. $C_7H_7NO_2$

m-Aminobenzoic acid
3-Amino-benzoesaeure
3-Aminobenzoic acid

RN: 99-05-8 **MP** (°C)**:** 174
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	5.900E+00	14.90	F300	1 0 0 0 1	
5.830E-02	7.995E+00	30	W007	2 0 2 2 2	

1140. $C_7H_7NO_2$
Methyl nicotinate
Nicotinsaeure-methyl ester
RN: 93-60-7 **MP** (°C)**:** 39
MW: 137.14 **BP** (°C)**:** 209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.471E-01	4.760E+01	20	F300	1 0 0 0 2	*sic*
8.065E+00	1.106E+03	32	L346	1 0 0 1 0	
3.467E-01	4.755E+01	ns	R424	0 0 0 0 0	

1141. $C_7H_7NO_2$
p-Nitrotoluene
4-Nitrotoluene
RN: 99-99-0 **MP** (°C)**:** 55
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	1.790E-01	9.99	B403	1 2 2 2 2	
2.917E-04	4.000E-02	14.5	D070	1 2 0 0 1	
2.917E-04	4.000E-02	14.50	F300	1 0 0 0 1	
1.765E-03	2.420E-01	19.99	B403	1 2 2 2 2	
2.100E-03	2.880E-01	20	H306	1 0 1 2 1	
2.150E-03	2.949E-01	20	T301	1 2 2 2 2	
2.348E-03	3.220E-01	29.99	B403	1 2 2 2 2	
3.048E-03	4.180E-01	39.99	B403	1 2 2 2 2	
5.687E-04	7.799E-02	50	D070	1 2 0 0 1	
8.458E-04	1.160E-01	100	D070	1 2 0 0 2	

1142. $C_7H_7NO_3$
3-Methyl-4-nitrophenol
3-Nitro-*p*-cresol
3-Nitro-*p*-kresol
4-Nitro-5-methylphenol
RN: 2581-34-2 **MP** (°C)**:** 128
MW: 153.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.769E-03	1.190E+00	25	B104	1 2 1 1 1	
7.762E-03	1.189E+00	ns	R427	0 0 0 0 0	

1143. $C_7H_7NO_3$
p-Aminosalicylic acid
4-Amino-salicylsaeure
4-Aminosalicylic acid
RN: 65-49-6 **MP** (°C)**:** 150
MW: 153.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	1.996E+00	20	D041	1 0 0 0 0	
1.100E-02	1.685E+00	23	M072	1 2 1 1 0	EFG
2.100E-02	3.216E+00	30	L069	1 0 1 1 0	EFG
1.087E-02	1.664E+00	ns	H125	0 0 0 0 0	

1144. $C_7H_7NO_3$
p-Nitroanisol
4-Nitro-anisol
4-Nitroanisol
RN: 100-17-4 **MP** (°C)**:** 54
MW: 153.14 **BP** (°C)**:** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	7.000E-02	15	F300	1 0 0 0 1	
3.853E-03	5.900E-01	30	F300	1 0 0 0 2	

1145. $C_7H_7N_2OS$
Ethyl acetylthiodiazole
Ethyle acetyle thiodiazolique
RN: **MP** (°C)**:**
MW: 167.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-03	2.000E-01	37	D084	1 0 1 0 1	

1146. $C_7H_7N_5$
2-Methylaminopteridine
Pteridine, 2-(methylamino)-
RN: 19167-57-8 **MP** (°C)**:** 219
MW: 161.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-02	3.115E+00	20	A019	2 2 1 1 1	
1.724E-01	2.778E+01	100	A019	1 2 1 1 1	

1147. C_7H_8
Toluene
Methylbenzene
RN: 108-88-3 **MP** (°C)**:** –94
MW: 92.14 **BP** (°C)**:** 110.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.819E-03	5.362E-01	.06	U010	1 0 0 1 1	EFG
7.857E-03	7.240E-01	0	P003	2 2 2 2 2	
6.638E-03	6.116E-01	4.50	B086	2 1 2 2 2	
5.557E-03	5.120E-01	4.62	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	4.62	U013	1 0 0 0 0	EFG
6.519E-03	6.006E-01	6.30	B086	2 1 2 2 2	
6.356E-03	5.857E-01	7.10	B086	2 1 2 2 2	
6.367E-03	5.867E-01	9	B086	2 1 2 2 2	
6.210E-03	5.722E-01	10	B149	2 1 1 2 2	
6.215E-03	5.727E-01	11.80	B086	2 1 2 2 2	
6.237E-03	5.747E-01	12.10	B086	2 1 2 2 2	
5.307E-03	4.890E-01	14.20	U013	1 0 0 0 0	EFG
5.785E-03	5.330E-01	15	S203	1 1 2 1 2	
6.172E-03	5.687E-01	15.10	B086	2 1 2 2 2	
5.424E-03	4.998E-01	16	D052	1 1 0 0 0	
5.100E-03	4.699E-01	16	F001	1 0 1 2 1	
5.101E-03	4.700E-01	16	F071	1 1 2 1 2	
5.101E-03	4.700E-01	16	F300	1 0 0 0 2	
5.101E-03	4.700E-01	16	H080	1 0 0 0 2	
5.100E-03	4.699E-01	16	S006	1 0 0 0 1	
6.370E-03	5.869E-01	20	B149	2 1 1 2 2	
6.154E-03	5.670E-01	20	B356	0 0 0 0 0	
5.424E-03	4.998E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
5.590E-03	5.151E-01	20	M312	1 0 0 0 2	
4.982E-03	4.591E-01	20	M337	2 1 2 2 2	
6.139E-03	5.657E-01	20.10	B086	2 1 2 2 2	
5.196E-03	4.788E-01	21	C024	2 1 1 2 2	
5.752E-03	5.300E-01	25	A001	1 2 2 2 1	
5.098E-03	4.698E-01	25	A094	1 0 0 0 1	
6.805E-03	6.270E-01	25	B003	2 1 2 2 2	
5.589E-03	5.150E-01	25	B060	2 0 1 1 1	
6.690E-03	6.164E-01	25	B153	2 1 1 1 2	
1.680E-02	1.548E+00	25	B173	2 0 2 2 2	*sic*
5.687E-03	5.240E-01	25	B304	2 0 2 2 2	
8.000E-03	7.371E-01	25	H092	1 1 1 1 0	
6.500E-03	5.989E-01	25	H313	2 1 2 2 1	
6.000E-03	5.529E-01	25	H332	2 2 2 2 0	
6.370E-02	5.869E+00	25	I334	2 2 2 1 2	*sic*
6.370E-03	5.869E-01	25	I335	2 2 2 2 2	
5.430E-03	5.003E-01	25	K001	1 0 2 1 2	
5.318E-03	4.900E-01	25	K072	1 0 1 1 1	
6.290E-03	5.796E-01	25	K316	2 2 2 2 2	
5.641E-03	5.197E-01	25	L319	1 0 2 1 2	

(*continued*)

1147. C_7H_8 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.589E-03	5.150E-01	25	M130	1 0 0 0 2	
5.638E-03	5.195E-01	25	M132	2 2 2 1 2	
6.280E-03	5.787E-01	25	M342	1 0 1 1 2	
6.219E-03	5.730E-01	25	P003	2 2 2 2 2	
6.012E-03	5.540E-01	25	P051	2 1 1 2 2	
6.045E-03	5.570E-01	25	S203	1 1 2 1 2	
5.804E-03	5.348E-01	25	S358	2 1 2 2 2	
5.650E-03	5.206E-01	25	S359	2 1 2 2 2	
6.280E-03	5.787E-01	25	W300	2 2 2 2 2	
5.307E-03	4.890E-01	25.35	U010	1 0 0 1 1	EFG
5.307E-03	4.890E-01	25.35	U013	1 0 0 0 0	EFG
3.255E-03	2.999E-01	30	F053	1 0 2 0 2	
6.183E-03	5.697E-01	30	G029	1 0 2 2 1	
5.067E-03	4.669E-01	30	M311	1 1 2 2 2	
1.409E-02	1.298E+00	30	S207	1 0 0 1 1	*sic*
5.557E-03	5.120E-01	34.53	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	34.53	U013	1 0 0 0 0	EFG
6.371E-03	5.870E-01	35	S203	1 1 2 1 2	
5.954E-03	5.486E-01	44.30	U010	1 0 0 1 1	EFG
5.819E-03	5.362E-01	44.30	U013	1 0 0 0 0	EFG
6.892E-03	6.350E-01	45	S203	1 1 2 1 2	
1.517E-02	1.398E+00	45	S207	1 0 0 1 1	*sic*
6.529E-03	6.015E-01	54.71	U013	1 0 0 0 0	EFG
1.500E-02	1.382E+00	55	H092	1 1 1 1 1	
6.380E-03	5.879E-01	55.79	U010	1 0 0 1 1	EFG
1.734E-02	1.597E+00	60	S207	1 0 0 1 1	*sic*
7.325E-03	6.749E-01	65.82	U013	1 0 0 0 0	EFG
2.171E-02	2.000E+00	150	J023	1 1 2 2 0	
7.597E-02	7.000E+00	200	J023	1 1 2 2 0	
3.039E-01	2.800E+01	250	J023	1 1 2 2 1	
1.411E+00	1.300E+02	300	J023	1 1 2 2 2	
5.589E-03	5.150E-01	ns	H123	0 0 0 0 0	
1.380E-01	1.272E+01	ns	H307	0 0 0 0 0	*sic*
5.611E-03	5.170E-01	ns	M175	0 0 2 1 2	
5.589E-03	5.150E-01	ns	M344	0 0 0 0 2	

1148. C_7H_8

1,6-Heptadiyne

RN: 2396-63-6 **MP** (°C)**:** –85
MW: 92.14 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.791E-02	1.650E+00	25	M001	2 1 2 2 2	

1149. C_7H_8
Cycloheptatriene
1,3,5-Cycloheptatriene
Tropilidene
CHT
RN: 544-25-2 **MP** (°C)**:** –80
MW: 92.14 **BP** (°C)**:** 116.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.301E-03	5.806E-01	4.8	L007	2 2 1 2 2	
6.301E-03	5.806E-01	5.1	L007	2 1 1 1 2	
7.207E-03	6.641E-01	14.8	L007	2 2 1 2 2	
7.207E-03	6.641E-01	15.2	L007	2 1 1 1 2	
7.260E-03	6.690E-01	24.8	L007	2 2 1 2 2	
6.729E-03	6.200E-01	25	M001	2 1 2 2 2	
7.260E-03	6.690E-01	25.1	L007	2 1 1 1 2	
8.045E-03	7.413E-01	34.8	L007	2 2 1 2 2	
8.045E-03	7.413E-01	35.2	L007	2 1 1 1 2	
8.294E-03	7.642E-01	44.8	L007	2 2 1 2 2	
8.294E-03	7.642E-01	45.2	L007	2 1 1 1 2	

1150. $C_7H_8ClN_3O_4S_2$
Hydrochlorothiazide
Chlorozide
RN: 58-93-5 **MP** (°C)**:** 274
MW: 297.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.425E-03	7.220E-01	25	A076	1 0 1 1 2	
2.032E-03	6.050E-01	25	C437	0 0 0 0 0	Average
2.045E-03	6.090E-01	25	D091	1 0 0 0 2	pH 6.2
2.687E-03	8.000E-01	25	G051	1 0 1 1 0	
2.800E-03	8.337E-01	30	A089	2 0 1 1 0	EFG
2.800E-03	8.337E-01	30	A093	2 0 1 1 0	EFG
2.520E-03	7.503E-01	30	E049	2 0 2 2 2	
3.627E-03	1.080E+00	37	D091	1 0 0 0 2	pH 7.2
7.650E-03	2.278E+00	50	M335	1 0 2 1 2	pH 5
3.359E-03	1.000E+00	ns	K444	0 0 0 0 0	
1.982E-03	5.900E-01	rt	A095	0 0 0 0 0	

1151. $C_7H_8ClN_3O_4S_2$

Hydrochlorothiazide
3,4-Dihydro-6-chloro-7-sulfamoyl-1,2,4-benzothiadiazine-1,1-dioxide
3,4-Dihydrochlorothiazide
6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide
6-Chloro-3,4-dihydro-7-sulfamoyl-2H-1,2,4-benzothiadiazine-1,1-dioxide
Aldactazide

RN: 58-93-5 **MP** (°C)**:** 274
MW: 297.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.946E-01	22.5	B422	2 0 2 2 2	
2.351E-06	7.000E-04	25	A408	2 0 1 2 0	
2.115E-03	6.296E-01	25	S450	0 0 0 0 0	

1152. $C_7H_8FN_3O_3$

1-Ethylcarbamoyl-5-fluorouracil
1-Ethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
N-Ethyl-5-fluoro-3,4-dihydro-2,4-dioxo-1-pyrimidinecarboxamide

RN: 58471-47-9 **MP** (°C)**:** 190–196
MW: 201.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.457E-03	1.500E+00	22	B321	0 0 0 0 0	pH 4.0
7.457E-03	1.500E+00	22	B388	0 0 0 0 0	

1153. $C_7H_8FN_3O_3$

1-(*N,N*-Dimethylcarbamoyl)-5-fluorouracil
1-Dimethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

RN: 60908-29-4 **MP** (°C)**:** 226–227
MW: 201.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.983E-02	6.000E+00	22	B321	0 0 0 0 0	pH 4.0
2.983E-02	6.000E+00	22	B388	0 0 0 0 0	

1154. $C_7H_8N_2O_2$

3-Nitro-*o*-toluidine
3-Nitro-*o*-toluidin

RN: 603-83-8 **MP** (°C)**:** 92
MW: 152.15 **BP** (°C)**:** 305

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.807E-02	1.340E+01	100	F300	1 0 0 0 2	

1155. $C_7H_8N_2O_3$
5,5-Trimethylenebarbituric acid
6,8-Diazaspiro[3.5]nonane-5,7,9-trione
Cyclobutane-spirobarbiturate
RN: 6128-03-6 **MP** (°C)**:**
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.213E-02	3.721E+00	25	P350	0 0 0 0 0	intrinsic

1156. $C_7H_8N_2O_3$
1-Methoxy-2-amino-4-nitrobenzene
RN: 99-59-2 **MP** (°C)**:** 118
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-03	5.697E-01	rt	N015	0 0 2 2 2	

1157. $C_7H_8N_2O_3S$
5-Carboethoxy-2-thiouracil
Ethyl 2-thiouracil-5-carboxylate
RN: 38026-46-9 **MP** (°C)**:** 252
MW: 200.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.970E-03	1.596E+00	25	G016	1 2 1 2 2	intrinsic

1158. $C_7H_8N_2O_4$
Ethyl orotate
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidine-carboxylic acid, ethyl ester
RN: 1747-53-1 **MP** (°C)**:**
MW: 184.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.867E+00	20	N019	0 0 0 0 0	

1159. $C_7H_8N_2S$
1-Phenyl-2-thiourea
Phenylthioharnstoff
RN: 103-85-5 **MP** (°C)**:** 149
MW: 152.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-02	2.600E+00	18	F300	1 0 0 0 1	
3.830E-01	5.830E+01	100	F300	1 0 0 0 2	

1160. $C_7H_8N_4O_2$
Theophylline
1,3-Dimethylxanthine
Aerolate
Bronkotabs
Bronchodid Duracap
Bronkodyl
RN: 58-55-9 **MP** (°C)**:** 272
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-02	5.964E+00	16	A072	1 0 1 0 1	
2.866E-02	5.164E+00	20	K052	1 1 1 1 2	
1.380E+00	2.486E+02	25	B443	0 0 0 0 0	
3.420E-02	6.162E+00	25	F009	2 2 2 2 0	EFG
3.675E-02	6.621E+00	25	L338	1 0 1 1 2	
4.089E-02	7.366E+00	25	M128	2 0 1 2 2	
4.083E-02	7.356E+00	25	M158	2 0 2 2 2	
3.580E-02	6.450E+00	25	N312	2 1 1 1 1	
4.607E-02	8.300E+00	25	P010	1 0 1 1 1	
4.607E-02	8.300E+00	25	P011	0 0 0 0 0	
4.440E-02	8.000E+00	25	P018	1 0 2 2 1	
4.440E-02	8.000E+00	25	P020	2 0 1 1 1	
4.607E-02	8.300E+00	25	P312	0 0 0 0 0	
4.500E-02	8.108E+00	30	B042	1 2 1 1 1	
4.500E-02	8.108E+00	30	G021	1 0 0 0 2	
4.100E-02	7.387E+00	30	H016	2 2 2 2 0	EFG
4.500E-02	8.108E+00	30	H020	1 0 0 0 1	
5.550E-02	1.000E+01	37	F076	2 0 2 2 0	
2.761E-02	4.975E+00	ns	J025	0 0 0 0 2	
5.550E-03	1.000E+00	ns	K444	0 0 0 0 0	
3.580E-02	6.450E+00	ns	N062	2 0 1 2 2	
2.054E-04	3.700E-02	rt	N015	0 0 2 2 1	*sic*

1161. $C_7H_8N_4O_2$
Theobromine
Theobromin
RN: 83-67-0 **MP** (°C)**:** 357
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.665E-03	3.000E-01	18	F300	1 0 0 0 0	
3.328E-03	5.996E-01	19	A072	1 0 1 0 0	
2.419E-03	4.358E-01	20	K052	1 1 1 1 2	
1.830E-03	3.297E-01	25	M158	2 0 2 2 2	
1.832E-03	3.300E-01	25	O302	1 0 0 1 0	
2.775E-03	5.000E-01	25	P010	1 0 1 1 1	
3.330E-03	6.000E-01	25	P011	0 0 0 0 0	
3.386E-03	6.100E-01	25	P018	1 0 2 2 1	

(*continued*)

1161. $C_7H_8N_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.108E-03	5.600E-01	25	P020	2 0 1 1 1	
3.000E-03	5.405E-01	30	B042	1 2 1 1 0	
~3.00E-03	~5.41E-01	30	H020	1 0 0 0 0	
3.830E-02	6.900E+00	100	F300	1 0 0 0 1	
2.774E-03	4.998E-01	c	D004	0 0 0 0 0	
3.676E-02	6.623E+00	h	D004	0 0 0 0 0	
>2.77E-03	>5.00E-01	ns	B404	0 2 1 1 0	

1162. C_7H_8O

p-Cresol
4-Cresol
p-Methylphenol

RN: 106-44-5 **MP** (°C)**:** 35.5
MW: 108.14 **BP** (°C)**:** 201.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.813E-01	1.961E+01	20	B031	1 0 2 2 1	
1.701E-01	1.840E+01	20	R087	0 0 0 0 0	0.15M NaCl
1.990E-01	2.152E+01	25	A021	1 2 1 1 0	
1.902E-01	2.057E+01	25	B019	1 0 1 2 0	
1.813E-01	1.961E+01	25	L022	1 0 0 0 0	
1.967E-01	2.127E+01	25	P004	0 0 0 0 0	
1.902E-01	2.057E+01	25	R041	0 0 0 0 0	
2.044E-01	2.210E+01	29.5	K119	1 0 0 0 2	
1.999E-01	2.162E+01	29.50	M098	1 2 0 1 2	
2.090E-01	2.260E+01	40	F300	1 0 0 0 2	
3.334E-01	3.605E+01	82.10	M098	1 2 0 1 2	

1163. C_7H_8O

Anisole
Methoxybenzene
Methyl phenyl ether
Phenyl methyl ether

RN: 100-66-3 **MP** (°C)**:** –37.3
MW: 108.14 **BP** (°C)**:** 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.295E-03	1.400E-01	25	A003	1 2 1 2 1	*sic*
9.609E-02	1.039E+01	25	B019	1 0 1 2 0	
1.000E-02	1.081E+00	25	D407	1 0 2 2 2	
1.400E-02	1.514E+00	25	M327	1 0 0 1 2	
1.418E-02	1.533E+00	25.04	V013	2 2 2 2 2	
9.617E-02	1.040E+01	26.70	L095	2 2 1 1 2	

1164. C_7H_8O

2-Cresol
2-Methylphenol
Phenol, 2-methyl-
o-Cresol
o-Methylphenol

RN: 95-48-7 **MP** (°C)**:** 31
MW: 108.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.519E-01	2.724E+01	20	B031	1 0 2 2 1	
2.276E-01	2.461E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.312E-01	2.500E+01	23	P332	0 0 0 0 0	
2.400E-01	2.595E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.127E-01	2.300E+01	25	B060	2 0 1 1 1	
2.400E-01	2.595E+01	25	B316	0 0 0 0 0	
2.300E-01	2.487E+01	25	F044	1 0 0 0 1	
2.423E-01	2.620E+01	25	F300	1 0 0 0 2	
2.569E-01	2.778E+01	25	L022	1 0 0 0 0	
2.999E-01	3.244E+01	25	P004	0 0 0 0 0	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
1.991E-01	2.153E+01	31	B092	2 1 1 1 2	
2.606E-01	2.818E+01	46.20	M098	1 2 0 1 1	
2.497E-01	2.700E+01	50	K119	1 0 0 0 2	
2.763E-01	2.988E+01	60	B092	2 1 1 1 2	
3.557E-01	3.846E+01	86.70	M098	1 2 0 1 1	
2.291E-01	2.477E+01	ns	R427	0 0 0 0 0	

1165. C_7H_8O

m-Cresol
3-Cresol
m-Methylphenol

RN: 108-39-4 **MP** (°C)**:** 11
MW: 108.14 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-01	1.147E+01	0	M041	1 1 0 0 2	
2.167E-01	2.344E+01	20	B031	1 2 2 2 1	
2.112E-01	2.284E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.149E-01	2.324E+01	20.3	L339	2 0 2 2 2	
1.420E-01	1.536E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.053E-01	2.220E+01	25	C060	1 2 1 1 2	
2.099E-01	2.270E+01	25	F300	1 0 0 0 2	
1.946E-01	2.105E+01	25	M041	1 1 0 0 2	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
2.292E-01	2.478E+01	40.0	L339	2 0 2 2 2	

(*continued*)

1165. C_7H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-01	2.900E+01	46.2	K119	1 0 0 0 2	
2.326E-01	2.515E+01	50	M041	1 1 0 0 2	
2.431E-01	2.629E+01	50.80	M098	1 2 0 1 1	
2.712E-01	2.933E+01	58.4	L339	2 0 2 2 2	
2.693E-01	2.913E+01	60	B031	1 2 2 2 1	
3.331E-01	3.602E+01	77.2	L339	2 0 2 2 2	
3.213E-01	3.475E+01	78.70	M098	1 2 0 1 1	
3.982E-01	4.306E+01	92.20	M098	1 2 0 1 1	
4.387E-01	4.744E+01	98.1	L339	2 0 2 2 2	

1166. C_7H_8O

Benzyl alcohol
Benzylalkohol
Benzenemethanol
Phenylmethanol
Phenylcarbinol
α-Hydroxytoluene

RN: 100-51-6 **MP** (°C)**:** –15.2
MW: 108.14 **BP** (°C)**:** 204.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.606E-01	3.900E+01	17	F300	1 0 0 0 1	
3.488E-01	3.772E+01	20	H044	1 0 2 1 2	
3.520E-01	3.807E+01	20	S006	1 0 0 0 2	
3.967E-01	4.290E+01	25	B304	2 0 2 2 2	
3.540E-01	3.828E+01	25	H044	1 0 2 1 2	
4.260E-01	4.607E+01	25	L322	1 1 2 2 1	
3.616E-01	3.911E+01	30	H044	1 0 2 1 2	
3.646E-01	3.943E+01	35	H044	1 0 2 1 2	
3.676E-01	3.975E+01	40	H044	1 0 2 1 2	
3.724E-01	4.027E+01	45	H044	1 0 2 1 2	
3.722E-01	4.025E+01	50	H044	1 0 2 1 2	
3.868E-01	4.182E+01	55	H044	1 0 2 1 2	

1167. $C_7H_8O_2$

Salicyl alcohol
Salicylalkohol

RN: 90-01-7 **MP** (°C)**:** 86
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.075E-01	6.300E+01	22	F300	1 0 0 0 1	

1168. $C_7H_8O_2$
Guaiacol
o-Methoxyphenol
RN: 90-05-1 **MP** (°C)**:** 28
MW: 124.14 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-01	1.870E+01	15	F300	1 0 0 0 2	
1.880E-01	2.334E+01	24.99	B353	0 0 0 0 0	
1.060E-02	1.316E+00	37	E028	1 0 1 1 2	*sic*
1.288E-03	1.599E-01	ns	R424	0 0 0 0 0	

1169. $C_7H_8O_2$
3-Methoxyphenol
Resorcinol monomethylether
p-Methoxyphenol
RN: 150-19-6 **MP** (°C)**:**
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-01	3.861E+01	25	B314	0 0 0 0 0	
3.110E-01	3.861E+01	30	B315	0 0 0 0 0	
4.000E-03	4.966E-01	37	E028	1 0 1 1 1	*sic*
4.966E-01	6.165E+01	ns	S460	0 0 0 0 0	

1170. $C_7H_8O_2$
p-Methoxyphenol
p-Hydroxyanisole
Hydroquinone monomethyl ether
4-Methoxyphenol
RN: 150-76-5 **MP** (°C)**:** 52.5
MW: 124.14 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-01	2.573E+01	20	R087	0 0 0 0 0	0.15M NaCl

1171. $C_7H_8O_2$

4,6-Dimethyl-1,2-pyrone
4,6-Dimethyl-α-pyrone
2,4-Dimethyl-α-pyrone
Mesitene lactone
4,6-Dimethyl-2-pyranone
4,6-Dimethyl-2H-pyran-2-one

RN: 675-09-2 **MP** (°C)**:** 49
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E+00	2.424E+02	59.7	W022	2 2 1 1 0	EFG
2.088E+00	2.593E+02	86.3	W022	2 2 1 1 0	EFG

1172. $C_7H_8O_3S$

p-Toluenesulfonic acid
4-Methylbenzenesulfonic acid
Methylbenzenesulfonic acid
Tosic acid
PTSA
Toluene-4-sulfonic acid

RN: 104-15-4 **MP** (°C)**:** 106.5
MW: 172.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E+00	4.993E+02	36.5	T023	1 2 2 1 2	
2.902E+00	4.997E+02	40.5	T023	1 2 2 1 2	
2.903E+00	4.999E+02	42.5	T023	1 2 2 1 2	

1173. $C_7H_8O_3S.H_2O$

p-Toluenesulfonic acid (monohydrate)

RN: 6192-52-5 **MP** (°C)**:** 104.5
MW: 190.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.008E+02	–6.5	T023	1 2 2 1 2	
2.120E+00	4.033E+02	–1.5	T023	1 2 2 1 2	
2.129E+00	4.050E+02	1.5	T023	1 2 2 1 2	
2.168E+00	4.125E+02	20.1	T023	1 2 2 1 2	
2.210E+00	4.203E+02	38.8	T023	1 2 2 1 2	
2.616E+00	4.975E+02	45.3	T023	1 2 2 1 2	
2.257E+00	4.293E+02	55.2	T023	1 2 2 1 2	
2.593E+00	4.933E+02	73.9	T023	1 2 2 1 2	
2.329E+00	4.431E+02	78.4	T023	1 2 2 1 2	
2.566E+00	4.882E+02	89.1	T023	1 2 2 1 2	
2.375E+00	4.517E+02	89.9	T023	1 2 2 1 2	

(*continued*)

1173. $C_7H_8O_3S.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.446E+00	4.652E+02	101.1	T023	1 2 2 1 2	
2.525E+00	4.802E+02	102.9	T023	1 2 2 1 2	
2.498E+00	4.751E+02	104.8	T023	1 2 2 1 2	

1174. $C_7H_8O_3S.2H_2O$

o-Toluenesulfonic acid (dihydrate)

RN: 68066-37-5 **MP** (°C)**:**

MW: 208.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E+00	3.577E+02	–25.0	T023	1 2 2 1 2	
1.773E+00	3.691E+02	–13.0	T023	1 2 2 1 2	
1.823E+00	3.795E+02	.8	T023	1 2 2 1 2	
1.891E+00	3.938E+02	16.8	T023	1 2 2 1 2	
1.954E+00	4.068E+02	31.2	T023	1 2 2 1 2	
2.264E+00	4.715E+02	48.2	T023	1 2 2 1 2	
2.055E+00	4.279E+02	50.0	T023	1 2 2 1 2	
2.243E+00	4.671E+02	54.0	T023	1 2 2 1 2	
2.090E+00	4.353E+02	56.0	T023	1 2 2 1 2	
2.207E+00	4.597E+02	60.4	T023	1 2 2 1 2	
2.148E+00	4.472E+02	61.2	T023	1 2 2 1 2	
2.179E+00	4.538E+02	62.0	T023	1 2 2 1 2	

1175. $C_7H_8O_3S.4H_2O$

p-Toluenesulfonic acid (tetrahydrate)

RN: 104-15-4 **MP** (°C)**:**

MW: 244.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E+00	3.473E+02	–27.0	T023	1 2 2 1 2	
1.437E+00	3.510E+02	–26.0	T023	1 2 2 1 2	
1.450E+00	3.543E+02	–18.5	T023	1 2 2 1 2	
1.527E+00	3.730E+02	–16.5	T023	1 2 2 1 2	
1.592E+00	3.888E+02	–10.5	T023	1 2 2 1 2	
1.613E+00	3.939E+02	–8.5	T023	1 2 2 1 2	
1.640E+00	4.005E+02	–7.0	T023	1 2 2 1 2	
1.576E+00	3.848E+02	–5.9	T023	1 2 2 1 2	
1.605E+00	3.921E+02	–3.4	T023	1 2 2 1 2	
1.622E+00	3.961E+02	–2.2	T023	1 2 2 1 2	
1.641E+00	4.008E+02	–1.0	T023	1 2 2 1 2	

1176. $C_7H_8O_7$
Methylenecitric acid
Methylen-citronensaeure
RN: 144-16-1 **MP** (°C)**:**
MW: 204.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-01	4.770E+01	20	F300	1 0 0 0 2	

1177. $C_7H_9ClN_2OS$
TO-2
5-Chloro-4-methyl-2-propionamide-thiazole
CMPT
RN: 13915-79-2 **MP** (°C)**:** 159
MW: 204.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.794E-04	1.800E-01	ns	M061	0 0 0 0 2	

1178. C_7H_9N
4-Ethylpyridine
4-Aethyl-pyridin
RN: 536-75-4 **MP** (°C)**:** –90.5
MW: 107.16 **BP** (°C)**:** 168.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.906E+00	4.186E+02	–19	C047	2 2 0 0 1	
2.495E+00	2.674E+02	182	C047	2 2 0 0 2	

1179. C_7H_9N
m-Toluidine
3-Toluidine
4-Methylaniline
p-Toluidine
p-Toluidin
RN: 106-49-0 **MP** (°C)**:** 43
MW: 107.16 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.066E-02	6.500E+00	15	F300	1 0 0 0 1	
6.026E-02	6.457E+00	20	B179	0 0 0 0 0	
3.890E-01	4.169E+01	20	B179	0 0 0 0 0	
1.403E-01	1.503E+01	20	C113	1 0 2 1 2	
6.200E-02	6.644E+00	20	H306	1 0 1 2 1	
6.119E-02	6.557E+00	20	T301	1 2 2 2 2	

1180. C_7H_9N
Methylaniline
N-Methylaniline
RN: 100-61-8 **MP** (°C)**:** –57
MW: 107.16 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.248E-02	5.624E+00	25	C113	1 0 2 1 2	

1181. C_7H_9N
3,4-Lutidine
3,4-Dimethylpyridine
RN: 583-58-4 **MP** (°C)**:** –12
MW: 107.16 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E+00	1.968E+02	–3.6	C047	2 2 0 0 2	
2.470E+00	2.647E+02	163	C047	2 2 0 0 1	
+2.29E+00	+2.45E+02	ns	S460	0 0 0 0 0	

1182. C_7H_9N
o-Toluidine
2-Toluidine
RN: 95-53-4 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.524E-01	1.633E+01	20	C113	1 0 2 1 2	
1.577E-01	1.690E+01	20	K119	1 0 0 0 2	
1.381E-01	1.480E+01	25	F300	1 0 0 0 2	

1183. C_7H_9N
3-Ethylpyridine
3-Aethyl-pyridin
β-Lutidine
RN: 536-78-7 **MP** (°C)**:**
MW: 107.16 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	2.701E+02	196	C047	2 2 0 0 1	

1184. C_7H_9N
3,5-Lutidine
3,5-Dimethylpyridine
RN: 591-22-0 **MP** (°C)**:** –9
MW: 107.16 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	–12	C047	2 2 0 0 2	
2.520E+00	2.701E+02	192	C047	2 2 0 0 1	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1185. C_7H_9N
2,6-Lutidine
2,6-Dimethyl-pyridin
2,6-Dimethylpyridine
RN: 108-48-5 **MP** (°C)**:** –6
MW: 107.16 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E+00	2.308E+02	34	C047	2 2 0 0 1	
2.714E+00	2.908E+02	231	C047	2 2 0 0 1	
+2.82E+00	+3.02E+02	ns	S460	0 0 0 0 0	

1186. C_7H_9N
2,5-Lutidine
2,5-Dimethyl-pyridin
2,5-Dimethylpyridine
RN: 589-93-5 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.984E+00	2.126E+02	13.1	C047	2 2 0 0 1	
7.186E-01	7.700E+01	23	F300	1 0 0 0 1	
2.570E+00	2.754E+02	207	C047	2 2 0 0 1	

1187. C_7H_9N
2,4-Lutidine
2,4-Dimethyl-pyridin
2,4-Dimethylpyridine
RN: 108-47-4 **MP** (°C)**:** –60
MW: 107.16 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.961E+00	4.245E+02	23	J007	1 2 0 1 2	average of 2
1.896E+00	2.032E+02	23.4	C047	2 2 0 0 2	

(*continued*)

1187. C_7H_9N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	23.40	A009	1 2 1 1 2	LCST
1.287E+00	1.379E+02	24.40	A009	1 2 1 1 2	EFG, LCST
2.419E+00	2.593E+02	25	A009	1 2 1 1 2	EFG, LCST
3.316E+00	3.553E+02	27.2	J007	1 2 0 1 2	
8.484E-01	9.091E+01	30	A009	1 2 1 1 2	EFG, LCST
3.111E+00	3.333E+02	32.50	A009	1 2 1 1 2	EFG, LCST
4.497E+00	4.819E+02	35.0	J007	1 2 0 1 2	
2.902E+00	3.110E+02	39.0	J007	1 2 0 1 2	
6.105E-01	6.542E+01	40	A009	1 2 1 1 2	EFG, LCST
3.500E+00	3.750E+02	50	A009	1 2 1 1 2	EFG, LCST
2.545E+00	2.727E+02	53	J007	1 2 0 1 2	
4.548E+00	4.873E+02	54.3	J007	1 2 0 1 2	
3.777E+00	4.048E+02	62.50	A009	1 2 1 1 2	EFG, LCST
2.204E+00	2.362E+02	68.5	J007	1 2 0 1 2	
6.105E-01	6.542E+01	149	A009	1 2 1 1 2	EFG, UCST
3.794E+00	4.065E+02	165	A009	1 2 1 1 2	EFG, UCST
1.287E+00	1.379E+02	180	A009	1 2 1 1 2	EFG, UCST
3.500E+00	3.750E+02	180	A009	1 2 1 1 2	EFG, UCST
3.111E+00	3.333E+02	186	A009	1 2 1 1 2	EFG, UCST
1.896E+00	2.032E+02	187	A009	1 2 1 1 2	EFG, UCST
2.419E+00	2.593E+02	187	A009	1 2 1 1 2	EFG, UCST
2.520E+00	2.701E+02	189	A009	1 2 1 1 2	UCST
2.520E+00	2.701E+02	189	C047	2 2 0 0 1	

1188. C_7H_9N

2,3-Lutidine
2,3-Dimethylpyridine

RN: 583-61-9 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.926E+00	2.063E+02	16.5	C047	2 2 0 0 1	
2.594E+00	2.780E+02	193	C047	2 2 0 0 2	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1189. C_7H_9N

2-Ethylpyridine
α-Lutidine

RN: 100-71-0 **MP** (°C)**:**
MW: 107.16 **BP** (°C)**:** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E+00	2.537E+02	–5	C047	2 2 0 0 1	
2.760E+00	2.958E+02	231	C047	2 2 0 0 1	
+3.24E+00	+3.47E+02	ns	S460	0 0 0 0 0	

1190. C_7H_9NO
p-Anisidine
4-Methoxybenzenamine
p-Methoxyaniline
4-Methoxy-1-aminobenzene
p-Methoxyphenylamine
RN: 104-94-9 **MP** (°C)**:** 57
MW: 123.16 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-02	1.147E+01	20	T301	1 2 2 2 2	

1191. C_7H_9NO
p-Tolylhydroxylamine
p-Tolylhydroxylamin
RN: 623-10-9 **MP** (°C)**:**
MW: 123.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-02	1.000E+01	5	F300	1 0 0 0 1	
4.027E-01	4.960E+01	100	F300	1 0 0 0 2	

1192. C_7H_9NO
o-Anisidine
2-Anisidine
2-Methoxybenzenamine
o-Methoxyaniline
2-Methoxy-1-aminobenzene
o-Methoxyphenylamine
RN: 90-04-0 **MP** (°C)**:** 5
MW: 123.16 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-01	1.264E+01	25	B019	1 0 1 2 0	

1193. $C_7H_9NO_2$
1,2-Dimethyl-3-hydroxy-4-pyridone
DMHP
RN: 30652-11-0 **MP** (°C)**:** 271–273
MW: 139.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-01	1.572E+01	25	C340	0 0 0 0 0	pH 9.4

1194. $C_7H_9NO_2S$
p-Toluenesulfonamide
p-Methylbenzenesulfonamide
4-Methylbenzenesulfonamide
RN: 70-55-3 **MP** (°C)**:** 138
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.900E+00	9	F300	1 0 0 0 1	
1.180E-02	2.020E+00	15	K024	1 2 1 1 2	
1.843E-02	3.156E+00	25	H105	1 1 0 1 2	

1195. $C_7H_9NO_2S$
o-Toluenesulfonamide
o-Methylbenzenesulfonamide
RN: 88-19-7 **MP** (°C)**:** 156
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.840E-03	1.000E+00	9	F300	1 0 0 0 0	
1.860E-02	3.185E+00	15	K024	1 2 1 1 2	
9.485E-03	1.624E+00	25	H105	1 1 0 1 2	

1196. $C_7H_9NO_2S$
m-Toluenesulfonamide
m-Methylbenzenesulfonamide
RN: 1899-94-1 **MP** (°C)**:**
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E-02	2.996E+00	15	K024	1 2 1 1 2	
4.563E-02	7.812E+00	25	H105	1 1 0 1 2	

1197. $C_7H_9NO_3S$
4-Amino-3-methylbenzene sulfonic acid
4-Amino-toluol-sulfosaeure-(3)
RN: 98-33-9 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.671E-02	5.000E+00	20	F300	1 0 0 0 0	

1198. $C_7H_9NO_3S$
4-Amino-2-methylbenzene sulfonic acid
4-Amino-toluol-sulfosaeure-(2)
RN: 133-78-8 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.404E-02	4.500E+00	20	F300	1 0 0 0 1	

1199. $C_7H_9NO_3S$
2-Amino-5-methylbenzene sulfonic acid
2-Amino-toluol-sulfosaeure-(5)
RN: 88-44-8 **MP** (°C)**:** >300
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	3.200E+01	19	F300	1 0 0 0 1	

1200. $C_7H_9NO_3S$
p-Methoxybenzenesulfonamide
4-Methoxybenzenesulfonamide
RN: 1129-26-6 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	2.921E+00	15	K024	1 2 1 1 2	

1201. $C_7H_9N_3O$
4-Phenylsemicarbazide
Phenylsemicarbazide
RN: 537-47-3 **MP** (°C)**:** 123.5
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
	6.995E-01	15	D068	1 2 0 0 0	

1202. $C_7H_9N_3O_2S_2$
Sulfathiourea
p-Aminobenzenesulfonylthiourea
p-Aminophenylsulfonylthiourea
Badional
Baldinol
Fontamide
RN: 515-49-1 **MP** (°C)**:** 171.5
MW: 231.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.365E-03	5.470E-01	20	F073	1 2 2 2 2	

1203. $C_7H_9N_3O_3$
Orotic acid ethylamide
RN: 1011-82-1 **MP** (°C)**:** 263–265
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.553E+01	–4	N018	0 0 0 0 0	
3.240E-01	5.935E+01	16	N018	0 0 0 0 0	
3.980E-01	7.290E+01	25	N018	0 0 0 0 0	

1204. $C_7H_9N_3O_3S$
Sulfanilylurea
Sulfanilylharnstoff
RN: 547-44-4 **MP** (°C)**:** 146
MW: 215.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.333E+00	20	F073	1 2 2 2 2	
5.575E-03	1.200E+00	37	F300	1 0 0 0 1	
5.012E-02	1.079E+01	ns	R427	0 0 0 0 0	

1205. $C_7H_9N_3O_4$
Orotic acid ethanol amide
RN: **MP** (°C)**:** 217–218
MW: 199.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-01	3.585E+01	–4	N018	0 0 0 0 0	
3.460E-01	6.891E+01	16	N018	0 0 0 0 0	
4.470E-01	8.903E+01	25	N018	0 0 0 0 0	

1206. $C_7H_9O_3P$

Hydroxymethylphenylphosphinic acid

RN: 61451-78-3 **MP** (°C)**:** 138
MW: 172.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E+02	2.007E+04	0	W422	0 0 0 0 0	
9.900E+00	1.704E+03	34.29	W422	0 0 0 0 0	
2.060E+01	3.546E+03	44.30	W422	0 0 0 0 0	
4.240E+01	7.298E+03	54.41	W422	0 0 0 0 0	
9.660E+01	1.663E+04	64.99	W422	0 0 0 0 0	
1.662E+02	2.861E+04	73.42	W422	0 0 0 0 0	
2.474E+02	4.258E+04	79.6	W422	0 0 0 0 0	
3.120E+02	5.370E+04	83.95	W422	0 0 0 0 0	

1207. C_7H_{10}

1,3-Cycloheptadiene

RN: 4054-38-0 **MP** (°C)**:**
MW: 94.16 **BP** (°C)**:** 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-03	6.192E-01	ns	S460	0 0 0 0 0	

1208. $C_7H_{10}N_2OS$

Propylthiouracil
6-Propyl-2-thiouracil
Propycil

RN: 51-52-5 **MP** (°C)**:** 220.0
MW: 170.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.520E-03	1.110E+00	20	A091	1 0 0 0 0	
6.455E-03	1.099E+00	20	I310	0 0 0 0 0	
7.070E-03	1.204E+00	25	G016	1 2 1 2 2	intrinsic
5.816E-02	9.901E+00	100	I310	0 0 0 0 0	
5.874E-03	1.000E+00	ns	K444	0 0 0 0 0	

1209. $C_7H_{10}N_2O_2S$

p-Methylaminobenzenesulfonamide
4-Methylaminobenzenesulfonamide

RN: 16891-79-5 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	9.312E-01	15	K024	1 2 1 1 2	

1210. $C_7H_{10}N_2O_2S$
*N*1-Methylsulfanilamide
4-Amino-*N*-methylbenzenesulfonamide
N-Methyl-*p*-aminobenzenesulfonamide
N-Methyl-4-aminobenzenesulfonamide
RN: 1709-52-0 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-02	1.760E+01	37	K095	2 0 0 0 2	intrinsic

1211. $C_7H_{10}N_2O_2S$
Toluenesulfamide
Sulfamide, (4-methylphenyl)-
p-Tolylsulfamide
RN: 15853-38-0 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	5.624E+00	37	A028	1 0 2 1 2	intrinsic

1212. $C_7H_{10}N_2O_3$
Isopropylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-
Isopropylbarbiturate
RN: 7391-69-7 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.482E-02	5.925E+00	20	J030	1 2 2 2 2	
5.905E-02	1.005E+01	37	J030	1 2 2 2 2	

1213. $C_7H_{10}N_2O_3$
5-Ethyl-5-methylbarbituric acid
5-Methyl-5-ethylbarbituric acid
RN: 27653-63-0 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.010E-02	1.363E+01	25	M310	2 2 2 2 2	
5.912E-02	1.006E+01	25	P350	0 0 0 0 0	intrinsic

1214. $C_7H_{10}N_4O_2S$

Sulfanilylguanidine
Sulfaguanidine
Sulfaguanidin
Sulfanilguanidin

RN: 57-67-0 **MP** (°C)**:** 190
MW: 214.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.131E-03	8.850E-01	20	F073	1 2 2 2 2	
4.663E-03	9.990E-01	25	D041	1 0 0 0 0	
8.868E-03	1.900E+00	37	R045	1 2 1 1 2	
1.025E-02	2.195E+00	37.50	M142	1 2 0 0 2	
4.201E-01	9.000E+01	h	F300	0 0 0 0 0	

1215. $C_7H_{10}N_4O_3.H_2O$

Theopylline (monohydrate)
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate

RN: 5967-84-0 **MP** (°C)**:** 269–272
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.823E-02	8.264E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

1216. $C_7H_{10}O_4S.H_2O$

o-Toluenesulfonic acid (monohydrate)
2-Methyl-benzenesulfonic acid (monohydrate)

RN: 88-20-0 **MP** (°C)**:**
MW: 208.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E+00	4.889E+02	32.5	T023	1 2 2 1 2	
2.335E+00	4.863E+02	38.6	T023	1 2 2 1 2	
2.318E+00	4.827E+02	45.7	T023	1 2 2 1 2	
2.266E+00	4.718E+02	48.5	T023	1 2 2 1 2	
2.302E+00	4.793E+02	48.6	T023	1 2 2 1 2	
2.273E+00	4.733E+02	49.0	T023	1 2 2 1 2	
2.289E+00	4.767E+02	49.6	T023	1 2 2 1 2	

1217. $C_7H_{10}O_5$
Shikimic acid
Shikimisaeure
RN: 138-59-0 **MP** (°C)**:** 190
MW: 174.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.613E-01	1.500E+02	21	F300	1 0 0 0 1	

1218. $C_7H_{10}O_5$
Mesoxalic acid diethyl ester
Mesooxalsaeure-diaethyl ester
RN: 609-09-6 **MP** (°C)**:** –30
MW: 174.15 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.249E+00	5.658E+02	22	F300	1 0 0 0 2	
+3.25E+00	+5.66E+02	ns	S460	0 0 0 0 0	

1219. $C_7H_{11}NO_2$
Ethosuximide
Zarontin
2-Ethyl-2-methylsuccinimide
RN: 77-67-8 **MP** (°C)**:**
MW: 141.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E+00	1.900E+02	25	P061	0 0 0 0 0	pH 3-7.9
7.084E-01	1.000E+02	ns	K444	0 0 0 0 0	

1220. $C_7H_{11}N_3O_2$
Ipronidazole
1-Methyl-2-isopropyl-5-nitro-imidazole
RN: 14885-29-1 **MP** (°C)**:** 58–60
MW: 169.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-02	9.400E+00	20	D344	0 0 0 0 0	
5.550E-02	9.390E+00	20	D344	0 0 0 0 0	
5.446E-02	9.214E+00	20	D344	0 0 0 0 0	
5.560E-02	9.407E+00	20	D344	0 0 0 0 0	

1221. $C_7H_{11}N_3O_2$
1-Methyl-L-histidine
L-1-Methylhistidine
RN: 15507-76-3 **MP** (°C)**:** >254
MW: 169.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.851E-01	1.667E+02	25	D041	1 0 0 0 0	

1222. $C_7H_{11}N_7S$
Aziprotryne
2-Azido-4-isopropylamino-6-methylmercapto-*s*-triazine
C-7019
RN: 4658-28-0 **MP** (°C)**:** 95
MW: 225.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-04	5.500E-02	20	M161	1 0 0 0 1	
3.329E-04	7.500E-02	ns	M061	0 0 0 0 1	

1223. C_7H_{12}
1,6-Heptadiene
RN: 3070-53-9 **MP** (°C)**:** –129.0
MW: 96.17 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.575E-04	4.400E-02	25	M001	2 1 2 2 1	

1224. C_7H_{12}
1-Heptyne
1-*n*-Heptyne
Pentylacetylene
Amylacetylene
RN: 628-71-7 **MP** (°C)**:** –81
MW: 96.17 **BP** (°C)**:** 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.774E-04	9.400E-02	25	M001	2 1 2 2 2	

1225. C_7H_{12}
Cycloheptene
(1Z)-Cycloheptene
cis-Cycloheptene
RN: 628-92-2 **MP** (°C)**:** –56
MW: 96.17 **BP** (°C)**:** 114.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-04	6.600E-02	25	M001	2 1 2 2 1	

1226. C_7H_{12}
1-Methyl-1-cyclohexene
1-Methylcyclohexene
RN: 591-49-1 **MP** (°C)**:** –120
MW: 96.17 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-04	5.200E-02	25	M001	2 1 2 2 2	

1227. C_7H_{12}
2-Heptyne
1-Methyl-2-butylacetylene
Butyl(methyl)acetylene
RN: 1119-65-9 **MP** (°C)**:**
MW: 96.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	1.635E-01	25	H039	1 2 2 2 2	

1228. C_7H_{12}
2-Methyl-3-hexyne
1-Ethyl-2-isopropylacetylene
RN: 36566-80-0 **MP** (°C)**:**
MW: 96.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	1.731E-01	25	H039	1 2 2 2 2	

1229. $C_7H_{12}BrNO_4$

5-Bromo-2-propyl-5-nitro-1,3-dioxane
2-Propyl-5-bromo-5-nitro-1,3-dioxane
RN: 53983-01-0 **MP** (°C)**:** 73–75
MW: 254.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-03	2.799E-01	25	L013	1 0 2 1 2	

1230. $C_7H_{12}ClN_5$

Norazine
2-Chloro-4-methylamino-6-isopropylamino-*s*-triazine
RN: 3004-71-5 **MP** (°C)**:** 157–159
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	20	J033	0 0 0 0 0	
1.289E-03	2.600E-01	21	B192	0 0 0 0 2	

1231. $C_7H_{12}ClN_5$

Simazine
2-Chloro-4-ethylamino-6-ethylamino-*s*-triazine
2-Chloro-4,6-bis(ethylamino)-*s*-triazine
Primatol S
RN: 122-34-9 **MP** (°C)**:** 224
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.918E-06	2.000E-03	10	B185	0 0 0 0 0	
2.512E-05	5.065E-03	20	B179	0 0 0 0 0	
2.479E-05	5.000E-03	20	B185	0 0 0 0 0	
2.827E-05	5.700E-03	20	C048	2 2 2 2 1	
1.736E-05	3.500E-03	20	F311	1 2 2 2 1	
2.479E-05	5.000E-03	21	B192	0 0 0 0 0	
2.479E-05	5.000E-03	21	G099	2 0 0 1 0	
2.479E-05	5.000E-03	22	M061	1 0 0 0 0	
7.500E-05	1.512E-02	26	G001	1 0 1 1 1	
1.310E-04	2.642E-02	50	G001	1 0 1 1 2	
4.165E-04	8.400E-02	85	B185	0 0 0 0 0	
4.110E-04	8.288E-02	85	B200	1 0 0 0 2	
1.736E-05	3.500E-03	ns	C101	0 0 0 0 1	
2.479E-05	5.000E-03	ns	G041	0 0 0 0 0	
2.479E-05	5.000E-03	ns	H112	0 0 0 0 0	
2.479E-05	5.000E-03	ns	J033	0 0 0 0 0	
3.074E-05	6.200E-03	ns	V414	0 0 0 0 0	
2.479E-05	5.000E-03	rt	M161	0 0 0 0 0	

1232. $C_7H_{12}ClN_5$
2-Chloro-4-methyl amino-6-propyl amino-*s*-triazine
1,3,5-Triazine-2,4-diamine, 6-chloro-*N*-methyl-*N′*-propyl-*s*-Triazine, 2-chloro-4-methylamino-6-propylamino-
RN: 73383-40-1 **MP** (°C)**:**
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	21	G099	2 0 0 1 0	

1233. $C_7H_{12}N_2O_2$
5-Isobutylhydantoin
Hydantoin of DL-leucine
RN: 67337-73-9 **MP** (°C)**:** 208
MW: 156.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.937E+00	ns	M025	0 2 0 1 2	

1234. $C_7H_{12}N_4O_5$
Diglycine hydantoic acid
Carbamidoglycylglycine
RN: **MP** (°C)**:** 194
MW: 232.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-01	2.926E+01	25	M024	1 2 0 1 2	

1235. $C_7H_{12}N_4O_5$
Carbamidodiglycylglycine
Triglycine hydantoin acid
RN: **MP** (°C)**:** 204
MW: 232.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.460E-02	1.036E+01	25	M024	1 2 0 1 2	

1236. $C_7H_{12}O$
3-Methylcyclohexanone
m-Methylcyclohexanone
RN: 591-24-2 **MP** (°C)**:** –75
MW: 112.17 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.335E-02	1.498E+00	20	D052	1 1 0 0 0	
1.349E-02	1.513E+00	ns	S460	0 0 0 0 0	

1237. $C_7H_{12}O$
2-Methylcyclohexanone
Methyl anone
o-Methylcyohexanone
Methyl cyclohexanone
RN: 583-60-8 **MP** (°C)**:**
MW: 112.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-01	1.274E+01	23.50	O005	2 0 2 2 2	

1238. $C_7H_{12}O_2$
Hexahydrobenzoic acid
Cyclohexanecarboxylic acid
Cyclohexan-carbonsaeure
RN: 98-89-5 **MP** (°C)**:** 31
MW: 128.17 **BP** (°C)**:** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.006E+00	15	L006	1 0 0 0 2	
1.560E-02	2.000E+00	21	F300	1 0 0 0 0	

1239. $C_7H_{12}O_2$
Isobutyl propenoate
2-methylpropyl acrylate
2-Propenoic acid, 2-methylpropyl ester
Acrylic acid isobutyl ester
Isobutyl 2-propenoate
Isobutyl acrylate
RN: 106-63-8 **MP** (°C)**:**
MW: 128.17 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.166E-02	7.903E+00	ns	S460	0 0 0 0 0	

1240. $C_7H_{12}O_4$
Pimelic acid
Heptanedioc acid
RN: 111-16-0 **MP** (°C)**:** 105.7
MW: 160.17 **BP** (°C)**:** 272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-01	1.786E+01	5.99	A341	0 0 0 0 0	
1.151E-01	1.844E+01	7.99	A341	0 0 0 0 0	
1.334E-01	2.137E+01	10.99	A341	0 0 0 0 0	
1.523E-01	2.439E+01	13	D041	1 0 0 0 1	
1.498E-01	2.400E+01	13.50	F300	1 0 0 0 1	
3.122E-01	5.000E+01	15	M051	1 0 0 0 1	
2.236E-01	3.582E+01	15.99	A341	0 0 0 0 0	
2.527E-01	4.048E+01	17.99	A341	0 0 0 0 0	
3.006E-01	4.815E+01	19.99	A341	0 0 0 0 0	
2.973E-01	4.762E+01	20	D041	1 0 0 0 0	
3.122E-01	5.000E+01	20	L041	1 0 0 1 1	
2.953E-01	4.730E+01	20	M171	1 0 0 0 1	
3.000E-02	4.805E+00	20	S006	1 0 0 0 1	
3.332E+00	5.337E+02	21	B040	1 0 1 1 2	*sic*
3.846E-01	6.160E+01	23.99	A341	0 0 0 0 0	
3.938E-01	6.307E+01	24.99	A341	0 0 0 0 0	
4.660E-01	7.464E+01	28.99	A341	0 0 0 0 0	
5.072E-01	8.124E+01	30.99	A341	0 0 0 0 0	
5.690E-01	9.114E+01	33.99	A341	0 0 0 0 0	
6.545E-01	1.048E+02	36.99	A341	0 0 0 0 0	
8.886E-01	1.423E+02	39.99	A341	0 0 0 0 0	
1.527E+00	2.446E+02	42.99	A341	0 0 0 0 0	
1.824E+00	2.922E+02	44.99	A341	0 0 0 0 0	
2.135E+00	3.420E+02	47.49	A341	0 0 0 0 0	
2.551E+00	4.086E+02	49.99	A341	0 0 0 0 0	
3.460E+00	5.542E+02	54.82	A341	0 0 0 0 0	
3.915E+00	6.270E+02	59.99	A341	0 0 0 0 0	
4.365E+00	6.991E+02	64.49	A341	0 0 0 0 0	
4.649E+00	7.446E+02	68.99	A341	0 0 0 0 0	
3.937E-01	6.306E+01	rt	H431	0 0 0 0 0	

1241. $C_7H_{12}O_4$
Diethyl malonate
Malonic
Malonic ester
Propanedioic acid diethyl ester
Ethyl propanedioate
Ethyl methane dicarboxylate
RN: 105-53-3 **MP** (°C)**:** –50
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E+00	6.169E+02	25	H430	0 0 0 0 0	
1.450E-01	2.322E+01	37	E028	1 0 1 1 2	

1242. $C_7H_{12}O_4$
Ethyl α-acetoxypropionate
Ethyl 2-(acetyloxy)propanoate
Ethyl 2-acetoxypropionate
RN: 2985-28-6 **MP** (°C)**:**
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.104E-01	3.370E+01	25	R006	2 2 0 1 2	

1243. $C_7H_{12}O_4$
3-Methyladipic acid
3-Methylhexanedioic acid
RN: 3058-01-3 **MP** (°C)**:** 101
MW: 160.17 **BP** (°C)**:** 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.986E-01	6.385E+01	9.50	A031	1 2 2 2 2	
4.732E-01	7.579E+01	12.80	A031	1 2 2 2 2	
1.241E+00	1.987E+02	25.90	A031	1 2 2 2 2	
1.865E+00	2.987E+02	29.80	A031	1 2 2 2 2	
2.531E+00	4.055E+02	33.20	A031	1 2 2 2 2	
3.707E+00	5.938E+02	41.10	A031	1 2 2 2 2	
4.663E+00	7.468E+02	52.30	A031	1 2 2 2 2	
5.340E+00	8.553E+02	64.30	A031	1 2 2 2 2	

1244. $C_7H_{12}O_4$

n-Butylmalonic acid
Acide *n*-butylmalonique
RN: 534-59-8 **MP** (°C)**:** 102
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-01	1.160E+02	0	M051	1 0 0 0 2	
1.898E+00	3.040E+02	15	M051	1 0 0 0 2	
2.735E+00	4.380E+02	25	M051	1 0 0 0 2	
4.951E+00	7.930E+02	50	M051	1 0 0 0 2	

1245. $C_7H_{12}O_5$

Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 176.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.214E-02	1.623E+01	25	R007	0 0 0 0 0	

1246. $C_7H_{12}O_6$

Quinic acid
Chinasaeure
D-(–)-Quinic acid
1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid
RN: 77-95-2 **MP** (°C)**:** 162
MW: 192.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E+00	2.900E+02	9	F300	1 0 0 0 1	

1247. $C_7H_{13}BrN_2O_2$

Carbromal
Adalin
Bromodiethylacetylurea
N-(Aminocarbonyl)-2-bromo-2-ethylbutanamide
1-Bromo-ethyl-butyryl-urea
Bromodiethylacetylcarbamide
RN: 77-65-6 **MP** (°C)**:** 117
MW: 237.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E-03	5.000E-01	20	F300	1 0 0 0 0	

1248. $C_7H_{13}BrN_2O_2$

Bromo-pivalate ureide

RN: **MP** (°C)**:**

MW: 237.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-01	5.123E+01	ns	F057	0 2 2 2 1	

1249. $C_7H_{13}NO_2S$

2-Ethyl-2-methyl-4-thiazolidinecarboxylic acid

4-Thiazolidinecarboxylic acid, 2-ethyl-2-methyl-

Thiazolidine-4-carboxylic acid, 2-ethyl-2-methyl-

RN: 56595-20-1 **MP** (°C)**:**

MW: 175.25 **BP** (°C)**:** 327.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-01	4.557E+01	21	B414	1 0 0 1 1	very fast and extent decompostion, uncertain value

1250. $C_7H_{13}NO_2S$

2-Propylthiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2-propyl-

RN: 4165-34-8 **MP** (°C)**:**

MW: 175.25 **BP** (°C)**:** 346.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-02	1.490E+01	21	B414	1 0 0 1 1	partial decomposition

1251. $C_7H_{13}NO_2S_2$

2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-dithiolane

1,3-Dithiolane-4-methanol, 2,2-dimethyl-, carbamate

RN: 35801-62-8 **MP** (°C)**:**

MW: 207.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.244E+00	rt	B174	0 0 1 0 0	

1252. $C_7H_{13}NO_3$
N-Formylleucine
N-Formyl-DL-leucine
RN: 6113-61-7 **MP** (°C)**:**
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-01	2.945E+01	ns	M025	0 2 0 1 2	

1253. $C_7H_{13}NO_3S$
2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-oxathiolane
1,3-Oxathiolane-5-methanol, 2,2-dimethyl-, carbamate
RN: 78002-88-7 **MP** (°C)**:**
MW: 191.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	5.738E+00	rt	B174	0 0 1 0 0	

1254. $C_7H_{13}N_3O_3S$
Oxamyl
Vydate
Thioxamyl
N′,N′-Dimethyl-*N*-[(methylcarbamoyl)oxy]-1-thiooxamimidic acid methyl ester
N,N-Dimethyl-α-methylcarbamoyloxyimino-α-(methylthio)acetamide
DPX 1410
RN: 23135-22-0 **MP** (°C)**:** 109
MW: 219.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E+00	2.825E+02	20	B179	0 0 0 0 0	
1.277E+00	2.800E+02	25	M161	1 0 0 0 2	
9.977E-01	2.188E+02	ns	H308	0 0 0 0 1	

1255. $C_7H_{13}N_5O$
Hydroxysimazine
1,3,5-Triazin-2(1H)-one, 4,6-bis(ethylamino)-
2-Hydroxysimazine
4,6-bis(Ethylamino)-*s*-triazin-2-ol
G 30414
RN: 2599-11-3 **MP** (°C)**:**
MW: 183.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.748E-02	2	B193	1 1 0 0 1	

1256. C_7H_{14}
1-Heptene
1-*n*-Heptene
n-Hept-1-ene
RN: 592-76-7 **MP** (°C)**:** –119
MW: 98.19 **BP** (°C)**:** 93.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	1.817E-02	25	M342	1 0 1 1 2	

1257. C_7H_{14}
2-Heptene
RN: 592-77-8 **MP** (°C)**:**
MW: 98.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-04	1.500E-02	23.5	S171	2 1 2 2 2	
1.528E-04	1.500E-02	25	M001	2 1 2 2 1	

1258. C_7H_{14}
Cycloheptane
RN: 291-64-5 **MP** (°C)**:** –12
MW: 98.19 **BP** (°C)**:** 118.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-04	1.820E-02	20	M337	2 1 2 2 2	
3.055E-04	3.000E-02	25	M001	2 1 2 2 2	
2.760E-04	2.710E-02	30	G313	2 1 1 2 2	

1259. C_7H_{14}
Methylcyclohexane
Hexahydrotoluene
Methyl cyclohexane
RN: 108-87-2 **MP** (°C)**:** –126
MW: 98.19 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-04	2.182E-02	2.34	S461	0 0 0 0 0	
2.000E-04	1.964E-02	9.99	S461	0 0 0 0 0	
1.711E-04	1.680E-02	20	B318	0 0 0 0 0	EFG
1.691E-04	1.660E-02	20	B356	0 0 0 0 0	
1.324E-04	1.300E-02	20	M337	2 1 2 2 2	
1.667E-04	1.636E-02	24.99	S461	0 0 0 0 0	
1.701E-04	1.670E-02	25	G313	2 1 1 2 2	
1.629E-04	1.600E-02	25	K119	1 0 0 0 2	

(*continued*)

1259. C_7H_{14} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	1.400E-02	25	M001	2 1 2 2 2	
1.426E-04	1.400E-02	25	M002	2 1 2 2 2	
1.629E-04	1.600E-02	25.0	P051	2 1 1 2 2	
1.629E-04	1.600E-02	25.00	P007	2 1 2 2 2	
1.644E-04	1.615E-02	26.1	M447	0 0 0 0 0	
1.375E-04	1.350E-02	28	B348	2 1 2 2 2	
1.833E-04	1.800E-02	40.1	P051	2 1 1 2 2	
1.833E-04	1.800E-02	40.10	P007	2 1 2 2 2	
1.925E-04	1.890E-02	55.7	P051	2 1 1 2 2	
1.925E-04	1.890E-02	55.70	P007	2 1 2 2 2	
2.800E-04	2.749E-02	70.5	M447	0 0 0 0 0	
3.442E-04	3.380E-02	99.1	P051	2 1 1 2 2	
3.442E-04	3.380E-02	99.10	P007	2 1 2 2 2	
5.589E-04	5.487E-02	100.5	M447	0 0 0 0 0	
8.097E-04	7.950E-02	120.0	P051	2 1 1 2 2	
8.097E-04	7.950E-02	120.00	P007	2 1 2 2 2	
1.355E-03	1.331E-01	131.0	M447	0 0 0 0 0	
1.416E-03	1.390E-01	137.3	P051	2 1 1 2 2	
1.416E-03	1.390E-01	137.30	P007	2 1 2 2 2	
2.485E-03	2.440E-01	149.5	P051	2 1 1 2 2	
2.485E-03	2.440E-01	149.50	P007	2 1 2 2 2	
2.349E-03	2.307E-01	151.4	M447	0 0 0 0 0	
1.426E-04	1.400E-02	ns	H123	0 0 0 0 0	

1260. $C_7H_{14}N_2O_2S$

Aldicarb
Temik
2-Methyl-2-(methylthio)propanal *O*-[(methylamino)carbonyl]oxime
UC 21149
N-Methylcarbamoyloxime,2-methyl-2-methylsulfenylpropionaldehyde
Methylcarbamic acid

RN: 116-06-3 **MP** (°C)**:** 99
MW: 190.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	6.017E+00	20	B179	0 0 0 0 0	
3.153E-02	6.000E+00	ns	H042	0 0 0 0 2	
3.135E-02	5.964E+00	ns	M061	0 0 0 0 0	
3.153E-02	6.000E+00	rt	M161	0 0 0 0 0	

1261. $C_7H_{14}N_2O_3$
ε-Aminocaproic hydantoic acid
ε-Uramidocaproic acid
RN: **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1262. $C_7H_{14}N_2O_3$
α-Aminocaproic hydantoic acid
α-Uramidocaproic acid
RN: **MP** (°C)**:** 169
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1263. $C_7H_{14}N_2O_4S_2$
Djenkoic acid
Djenkolsaeure
RN: 498-59-9 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-02	5.000E+00	100	F300	1 0 0 0 0	

1264. $C_7H_{14}N_6$
*N*2,*N*2,*N*4,*N*4-Tetramethylmelamine
Tetramethylmelamine
RN: 2827-47-6 **MP** (°C)**:** 227.0
MW: 182.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.052E-03	3.740E-01	25	C051	1 2 1 1 2	pH 7

1265. $C_7H_{14}O$
Cycloheptanol
RN: 502-41-0 **MP** (°C)**:**
MW: 114.19 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1266. $C_7H_{14}O$

Heptyl aldehyde
Heptanal
Oenanthaldehyd

RN: 111-71-7 **MP** (°C)**:** –43.3
MW: 114.19 **BP** (°C)**:** 152.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-02	3.100E+00	0	F300	1 0 0 0 1	
1.576E-02	1.800E+00	40	F300	1 0 0 0 1	

1267. $C_7H_{14}O$

4-Methyl-cyclohexanol

RN: 589-91-3 **MP** (°C)**:** –41
MW: 114.19 **BP** (°C)**:** 171–173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1268. $C_7H_{14}O$

Dipropyl ketone
4-Heptanone

RN: 123-19-3 **MP** (°C)**:** –32.6
MW: 114.19 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.430E-02	7.342E+00	0	G032	1 2 1 1 2	
4.660E-02	5.321E+00	10	G032	1 2 1 1 2	
3.750E-02	4.282E+00	20	D052	1 1 0 0 1	
2.793E-02	3.190E+00	25.50	O005	2 0 2 2 1	
3.350E-02	3.825E+00	30	G032	1 2 1 1 2	
2.880E-02	3.289E+00	50	G032	1 2 1 1 2	
2.720E-02	3.106E+00	75	G032	1 2 1 1 2	

1269. $C_7H_{14}O$

2-Heptanone
Heptan-2-one

RN: 110-43-0 **MP** (°C)**:** –31
MW: 114.19 **BP** (°C)**:** 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.489E-02	3.984E+00	20	D052	1 1 0 0 0	
3.836E-02	4.381E+00	20	G030	1 2 0 0 1	
3.800E-02	4.339E+00	20	M312	1 0 0 0 1	
3.750E-02	4.282E+00	25	G030	1 2 0 0 1	
1.675E-01	1.913E+01	25	P055	1 0 0 0 1	
3.570E-02	4.077E+00	25	W300	2 2 2 2 2	
3.489E-02	3.984E+00	30	G030	1 2 0 0 1	

1270. $C_7H_{14}O$
5-Methyl-2-hexanone
Methyl isoamyl ketone
Isopentyl methyl ketone
Methylhexanone
Methyl isoamyl ketone
MIAK
RN: 110-12-3 **MP** (°C)**:** –74
MW: 114.19 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.677E-02	5.341E+00	ns	S460	0 0 0 0 0	

1271. $C_7H_{14}O$
2,4-Dimethyl-3-pentanone
2,4-Dimethylpentanone-3
RN: 565-80-0 **MP** (°C)**:** –80
MW: 114.19 **BP** (°C)**:** 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.137E-02	5.865E+00	20	G030	1 2 0 0 1	
4.963E-02	5.668E+00	25	G030	1 2 0 0 1	
4.877E-02	5.569E+00	30	G030	1 2 0 0 1	
4.972E-02	5.677E+00	ns	J300	0 0 0 0 0	

1272. $C_7H_{14}O_2$
Heptoic acid
Heptanoic acid
n-Heptanoic acid
RN: 111-14-8 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-02	1.900E+00	0	B136	1 0 2 1 2	
1.843E-02	2.400E+00	15	F300	1 0 0 0 1	
1.847E-02	2.404E+00	15	L006	1 0 0 0 2	
1.721E-02	2.240E+00	20	B136	1 0 2 1 2	
1.870E-02	2.434E+00	20.0	R001	1 1 1 1 2	
2.161E-02	2.813E+00	25	H122	1 0 0 0 2	
2.082E-02	2.710E+00	30	B136	1 0 2 1 2	
2.076E-02	2.703E+00	30.0	R001	1 1 1 1 2	
2.389E-02	3.110E+00	45	B136	1 0 2 1 2	
2.381E-02	3.100E+00	45.0	R001	1 1 1 1 2	
2.711E-02	3.530E+00	60	B136	1 0 2 1 2	
2.702E-02	3.518E+00	60.0	R001	1 1 1 1 2	
1.457E-02	1.896E+00	.0	R001	1 1 1 1 2	

1273. $C_7H_{14}O_2$
Pentyl acetate
Amyl acetate
RN: 628-63-7 **MP** (°C)**:** –100
MW: 130.19 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-02	1.697E+00	20	D052	1 1 0 0 1	
1.290E-02	1.679E+00	20	S006	1 0 0 0 2	
1.329E-02	1.730E+00	25	K072	1 0 1 1 1	
1.329E-02	1.730E+00	25	M087	1 1 2 1 2	
3.060E-02	3.984E+00	30	R318	1 1 0 1 0	

1274. $C_7H_{14}O_2$
Isopropyl *N*-butyrate
Isopropyl butyrate
N-Butyric acid isopropyl ester
RN: 638-11-9 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-02	1.560E+00	ns	J300	0 0 0 0 0	

1275. $C_7H_{14}O_2$
3-Hydroxy-5-methyl-5-ethyltetrahydrofuran
3-Furanol, 5-ethyltetrahydro-5-methyl-
RN: 30010-08-3 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.983E-01	9.091E+01	rt	B066	0 2 0 0 1	

1276. $C_7H_{14}O_2$
Isoamyl acetate
Acetic acid isoamyl ester
Essigsaeureisoamyl ester
RN: 123-92-2 **MP** (°C)**:** –79
MW: 130.19 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	2.500E+00	15	F300	1 0 0 0 1	
1.222E-02	1.591E+00	20	E002	1 0 0 0 1	
1.227E-02	1.597E+00	23.50	O005	2 0 2 2 1	
1.533E-02	1.996E+00	25	L062	2 2 0 1 0	

1277. $C_7H_{14}O_2$
Methyl hexanoate
Methyl caproate
RN: 106-70-7 **MP** (°C)**:** –71.0
MW: 130.19 **BP** (°C)**:** 151.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E-02	1.325E+00	20	M337	2 1 2 2 2	

1278. $C_7H_{14}O_2$
Ethyl pentanoate
Ethyl *n*-valerate
Ethyl valerianate
RN: 539-82-2 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-02	2.226E+00	ns	S460	0 0 0 0 0	

1279. $C_7H_{14}O_2$
n-Butyl propionate
Butyl propionate
RN: 590-01-2 **MP** (°C)**:** –89
MW: 130.19 **BP** (°C)**:** 146.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-02	1.498E+00	20	D052	1 1 0 0 0	
9.500E-03	1.237E+00	25	K012	1 0 0 0 1	
1.514E-02	1.970E+00	ns	S460	0 0 0 0 0	

1280. $C_7H_{14}O_2$
Propyl butyrate
Buttersaeure-propyl ester
n-Propyl *n*-butyrate
RN: 105-66-8 **MP** (°C)**:** –95
MW: 130.19 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.614E+00	17	F001	1 0 1 0 2	
1.244E-02	1.620E+00	17	F300	1 0 0 0 2	
1.200E-02	1.562E+00	17	S006	1 0 0 0 1	

1281. $C_7H_{14}O_2$
sec-Amyl acetate
2-Pentyl acetate
1-Methylbutyl acetate
RN: 53496-15-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-02	1.896E+00	20	D052	1 1 0 0 0	

1282. $C_7H_{14}O_3$
n-Ethyl β-ethoxypropionate
Ethyl β-ethoxypropionate
RN: 763-69-9 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:** 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-01	5.258E+01	25	D002	1 2 1 1 2	
3.566E-01	5.213E+01	25	R034	0 0 0 0 1	

1283. $C_7H_{14}O_3$
Butyl lactate
Butyl α-hydroxypropionate
2-Propanoic acid
Lactic acid butyl ester
Butyl 2-hydroxypropanoate
RN: 138-22-7 **MP** (°C)**:** –28
MW: 146.19 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.631E-01	3.846E+01	20	D052	1 1 0 0 1	
2.982E-01	4.360E+01	25	R006	2 2 0 1 2	

1284. $C_7H_{14}O_3$
n-Propyl β-methoxypropionate
Propionic acid, 3-methoxy-, propyl ester
RN: 5349-56-4 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E-01	3.101E+01	25	R034	0 0 0 0 1	

1285. $C_7H_{14}O_3$
Methyl β-*n*-propoxypropionate
Propanoic acid, 3-propoxy-, methyl ester
RN: 14144-39-9 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.249E-01	3.288E+01	25	R034	0 0 0 0 1	

1286. $C_7H_{14}O_3$
3-Methoxy butyl acetate
3-Methoxy-1-butanol acetate
Methyl-1,3-butylene glycol acetate
3-Methoxybutyl acetate
Butoxyl
Butoxyl (3-methoxy-*N*-butyl acetate)
RN: 4435-53-4 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.151E-01	6.068E+01	20	D052	1 1 0 0 2	

1287. $C_7H_{14}O_6$
β-Methyl-D-glucoside
β-Methyl-D-glucosid
RN: 709-50-2 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.892E+00	3.674E+02	17	F300	1 0 0 0 2	

1288. $C_7H_{14}O_6$
α-D-Methylglucoside
α-Methyl-D-glucoside
α-Methyl-D-glucosid
RN: 97-30-3 **MP** (°C)**:** 168
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E+00	3.868E+02	17	F300	1 0 0 0 2	
2.543E+00	4.938E+02	17.8	W013	1 2 1 1 2	
2.637E+00	5.120E+02	22.5	W013	1 2 1 1 2	
2.657E+00	5.159E+02	25.5	W013	1 2 1 1 2	
2.696E+00	5.236E+02	26.6	W013	1 2 1 1 2	
2.699E+00	5.241E+02	27.3	W013	1 2 1 1 2	

(*continued*)

1288. $C_7H_{14}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.751E+00	5.342E+02	31.8	W013	1 2 1 1 2	
2.806E+00	5.448E+02	33.9	W013	1 2 1 1 2	
2.849E+00	5.533E+02	37.2	W013	1 2 1 1 2	
2.951E+00	5.731E+02	43.2	W013	1 2 1 1 2	
3.060E+00	5.942E+02	49.0	W013	1 2 1 1 2	
3.078E+00	5.978E+02	49.6	W013	1 2 1 1 2	
3.131E+00	6.079E+02	51.8	W013	1 2 1 1 2	
3.166E+00	6.148E+02	54.4	W013	1 2 1 1 2	
3.213E+00	6.240E+02	57.3	W013	1 2 1 1 2	
3.297E+00	6.402E+02	60.6	W013	1 2 1 1 2	
3.332E+00	6.471E+02	62.7	W013	1 2 1 1 2	
3.360E+00	6.525E+02	64.2	W013	1 2 1 1 2	
3.403E+00	6.608E+02	66.2	W013	1 2 1 1 2	
3.435E+00	6.670E+02	67.8	W013	1 2 1 1 2	
3.542E+00	6.878E+02	73.2	W013	1 2 1 1 2	
3.651E+00	7.090E+02	78.0	W013	1 2 1 1 2	

1289. $C_7H_{14}O_6$

α-Methyl-D-mannoside
α-Methyl-D-mannosid
RN: 617-04-9 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.976E+02	17	F300	1 0 0 0 2	

1290. $C_7H_{14}O_7$

D-Mannoheptose
D-Sedoheptose
RN: 7634-39-1 **MP** (°C)**:**
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.76E-01	>1.00E+02	20	F300	1 0 0 0 0	

1291. $C_7H_{14}O_7$

D-α-Glucoheptose
Gluco-heptose
RN: 62475-58-5 **MP** (°C)**:**
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	8.676E+01	20	D041	1 0 0 0 1	

1292. $C_7H_{15}Br$
1-Bromoheptane
Heptyl bromide
RN: 629-04-9 **MP** (°C)**:** –56.1
MW: 179.11 **BP** (°C)**:** 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-05	6.645E-03	25	M342	1 0 1 1 2	

1293. $C_7H_{15}Cl$
1-Chloroheptane
Heptyl chloride
RN: 629-06-1 **MP** (°C)**:** –69.5
MW: 134.65 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-04	1.360E-02	25	M342	1 0 1 1 2	

1294. $C_7H_{15}Cl_2N_2O_2P$
Cyclophosphamide
Cyclophosphoramide
2-(bis(2-Chloroethyl)-amino)tetrahydro-2H-1,3,2-oxazaphosphorine 2-oxide
Cycloblastin
Sendoxan
Claphene
RN: 50-18-0 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.532E-01	4.000E+01	ns	K444	0 0 0 0 0	

1295. $C_7H_{15}I$
1-Iodoheptane
Heptyl iodide
RN: 4282-40-0 **MP** (°C)**:** –48.2
MW: 226.10 **BP** (°C)**:** 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-05	3.505E-03	25	M342	1 0 1 1 2	

1296. $C_7H_{15}NO_2$
Isobutyl urethane
Isobutylurethan
RN: 539-89-9 **MP** (°C)**:**
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	2.482E+01	15.5	F001	1 0 1 2 2	

1297. $C_7H_{15}NO_2$
n-Hexyl carbamate
Hexyl carbamate
RN: 2114-20-7 **MP** (°C)**:** 62
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	1.742E+00	37	H006	1 2 2 1 1	

1298. $C_7H_{15}NO_2$
tert-Hexyl carbamate
3,3-Dimethyl-1-butanol carbamate
RN: 3124-38-7 **MP** (°C)**:**
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.937E+00	37	H006	1 2 2 1 1	

1299. C_7H_{16}
3,3-Dimethylpentane
3,3-Dwumetylopentan
RN: 562-49-2 **MP** (°C)**:** –135
MW: 100.21 **BP** (°C)**:** 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.928E-05	5.940E-03	25	K119	1 0 0 0 2	
5.908E-05	5.920E-03	25.0	P051	2 1 1 2 2	
5.908E-05	5.920E-03	25.00	P007	2 1 2 2 2	
6.766E-05	6.780E-03	40.1	P051	2 1 1 2 2	
6.766E-05	6.780E-03	40.10	P007	2 1 2 2 2	
8.153E-05	8.170E-03	55.7	P051	2 1 1 2 2	
8.153E-05	8.170E-03	55.70	P007	2 1 2 2 2	
1.028E-04	1.030E-02	69.7	P051	2 1 1 2 2	
1.028E-04	1.030E-02	69.70	P007	2 1 2 2 2	
1.577E-04	1.580E-02	99.1	P051	2 1 1 2 2	

(*continued*)

1299. C_7H_{16} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-04	1.580E-02	99.10	P007	2 1 2 2 2	
2.724E-04	2.730E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	118.00	P007	2 1 2 2 2	
6.716E-04	6.730E-02	120.4	P051	2 1 1 2 2	
6.716E-04	6.730E-02	120.40	P007	2 1 2 2 2	
8.592E-04	8.610E-02	150.4	P051	2 1 1 2 2	
8.592E-04	8.610E-02	150.40	P007	2 1 2 2 2	

1300. C_7H_{16}
3-Methylhexane
3-Metyloheksan
RN: 589-34-4 **MP** (°C)**:** –119
MW: 100.21 **BP** (°C)**:** 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.229E-05	5.240E-03	0	P003	2 2 2 2 2	
1.048E-04	1.050E-02	23	C332	0 0 0 0 0	
2.635E-05	2.640E-03	25	K119	1 0 0 0 2	
4.940E-05	4.950E-03	25	P003	2 2 2 2 2	
2.635E-05	2.640E-03	25	P051	2 1 1 2 2	
2.635E-05	2.640E-03	25.00	P007	2 1 2 2 2	

1301. C_7H_{16}
2,4-Dimethylpentane
2,4-Dwumetylopentan
RN: 108-08-7 **MP** (°C)**:** –123
MW: 100.21 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.487E-05	6.500E-03	0	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	K119	1 0 0 0 2	
4.052E-05	4.060E-03	25	M001	2 1 2 2 2	
3.613E-05	3.620E-03	25	M002	2 1 2 2 2	
5.489E-05	5.500E-03	25	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	P051	2 1 1 2 2	
4.401E-05	4.410E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1302. C_7H_{16}
2,3-Dimethylpentane
2,3-Dwumetylopentan
RN: 565-59-3 **MP** (°C)**:** <25
MW: 100.21 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.239E-05	5.250E-03	25	K119	1 0 0 0 2	
5.239E-05	5.250E-03	25	P051	2 1 1 2 2	
5.239E-05	5.250E-03	25.00	P007	2 1 2 2 2	

1303. C_7H_{16}
2-Methylhexane
2-Metyloheksan
RN: 591-76-4 **MP** (°C)**:** –118
MW: 100.21 **BP** (°C)**:** 90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	1.400E-02	23	C332	0 0 0 0 0	
2.535E-05	2.540E-03	25	K119	1 0 0 0 2	
2.535E-05	2.540E-03	25	P051	2 1 1 2 2	
2.535E-05	2.540E-03	25.00	P007	2 1 2 2 2	

1304. C_7H_{16}
2,2-Dimethylpentane
2,2-Dwumetylopentan
RN: 590-35-2 **MP** (°C)**:** –123
MW: 100.21 **BP** (°C)**:** 79.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.391E-05	4.400E-03	25	K119	1 0 0 0 2	
4.391E-05	4.400E-03	25	P051	2 1 1 2 2	
4.391E-05	4.400E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1305. C_7H_{16}
Heptane
n-Heptane
RN: 142-82-5 **MP** (°C)**:** –90.7
MW: 100.21 **BP** (°C)**:** 98.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.381E-05	4.390E-03	0	P003	2 2 2 2 2	
8.333E-05	8.350E-03	2.34	S461	0 0 0 0 0	

(*continued*)

1305. C_7H_{16} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-05	1.954E-03	4.3	N004	1 1 2 2 2	
1.667E-05	1.670E-03	9.99	S461	0 0 0 0 0	
2.017E-05	2.021E-03	13.5	N004	1 1 2 2 2	
4.990E-04	5.000E-02	15	F300	1 0 0 0 1	
5.200E-04	5.211E-02	15.50	F001	1 0 1 0 2	
1.497E-04	1.500E-02	16	D047	1 0 0 1 0	
2.694E-05	2.700E-03	20	M337	2 1 2 2 1	
1.111E-05	1.113E-03	24.99	S461	0 0 0 0 0	
3.990E-03	3.998E-01	25	G323	2 2 2 2 0	
4.990E-04	5.000E-02	25	K072	1 0 1 1 1	
2.235E-05	2.240E-03	25	K119	1 0 0 0 2	
2.924E-05	2.930E-03	25	M001	2 1 2 2 2	
2.924E-05	2.930E-03	25	M002	2 1 2 2 2	
4.990E-04	5.000E-02	25	M087	1 1 2 1 0	
3.050E-05	3.056E-03	25	M342	1 0 1 1 2	
3.363E-05	3.370E-03	25	P003	2 2 2 2 2	
4.989E-04	5.000E-02	25	S012	2 0 2 2 0	
2.656E-05	2.661E-03	25.0	N004	1 1 2 2 2	
2.235E-05	2.240E-03	25.0	P051	2 1 1 2 2	
2.235E-05	2.240E-03	25.00	P007	2 1 2 2 2	
2.261E-05	2.266E-03	35.0	N004	1 1 2 2 2	
2.625E-05	2.630E-03	40.1	P051	2 1 1 2 2	
2.400E-05	2.405E-03	45.0	N004	1 1 2 2 2	
8.973E-03	8.992E-01	50	G323	2 2 2 2 0	
3.104E-05	3.110E-03	55.7	P051	2 1 1 2 2	
3.104E-05	3.110E-03	55.70	P007	2 1 2 2 2	
5.589E-05	5.600E-03	99.1	P051	2 1 1 2 2	
5.589E-05	5.600E-03	99.10	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.6	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.60	P007	2 1 2 2 2	
4.361E-04	4.370E-02	150.4	P051	2 1 1 2 2	
4.361E-04	4.370E-02	150.40	P007	2 1 2 2 2	
3.692E-05	3.700E-03	ns	B151	0 2 1 1 1	
7.000E-04	7.014E-02	ns	H012	0 2 2 0 0	

1306. $C_7H_{16}O$

3-Heptanol
(±)-3-Heptanol
3-Hydroxyheptane
1-Ethyl-1-pentanol

RN: 589-82-2 **MP** (°C)**:** –70
MW: 116.20 **BP** (°C)**:** 156.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-02	4.764E+00	20	H330	0 0 0 0 0	
3.428E-02	3.984E+00	25	C093	2 1 1 1 0	

1307. $C_7H_{16}O$
2-Heptanol
2-Hydroxyheptane
Amylmethylcarbinol
RN: 543-49-7 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 159.00

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.532E-02	6.428E+00	0	S307	1 1 0 2 2	
3.966E-02	4.609E+00	10.2	S307	1 1 0 2 2	
3.633E-02	4.222E+00	19.5	S307	1 1 0 2 2	
3.001E-02	3.488E+00	30.7	S307	1 1 0 2 2	
2.813E-02	3.269E+00	40.0	S307	1 1 0 2 2	
2.514E-02	2.921E+00	50.0	S307	1 1 0 2 2	
2.471E-02	2.872E+00	60.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	70.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	80.0	S307	1 1 0 2 2	
2.942E-02	3.418E+00	90.2	S307	1 1 0 2 2	

1308. $C_7H_{16}O$
3-Methyl-3-hexanol
3-Methylhexanol-3
RN: 597-96-6 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.146E-01	1.332E+01	20	G006	1 2 1 1 2	
1.012E-01	1.176E+01	25	G006	1 2 1 1 2	
9.110E-02	1.059E+01	30	G006	1 2 1 1 2	

1309. $C_7H_{16}O$
3-Ethyl-3-pentanol
3-Ethyl-pentanol-3
Triethyl carbinol
RN: 597-49-9 **MP** (°C)**:** –12
MW: 116.20 **BP** (°C)**:** 141.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-01	1.874E+01	20	G006	1 2 1 1 2	
1.422E-01	1.652E+01	25	G006	1 2 1 1 2	
1.272E-01	1.478E+01	30	G006	1 2 1 1 2	
1.071E-01	1.244E+01	40	G006	1 2 1 1 2	

1310. $C_7H_{16}O$

2-Methyl-2-hexanol
2-Methylhexanol-2
RN: 625-23-0 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.195E-02	1.068E+01	20	G006	1 2 1 1 2	
8.267E-02	9.607E+00	25	G006	1 2 1 1 1	
7.422E-02	8.625E+00	30	G006	1 2 1 1 1	

1311. $C_7H_{16}O$

2,4-Dimethyl-3-pentanol
2,4-Dimethylpentanol-3
Diisopropyl carbinol
RN: 600-36-2 **MP** (°C)**:** –70
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.172E+01	0	S307	1 1 0 2 2	
8.942E-02	1.039E+01	10.0	S307	1 1 0 2 2	
6.660E-02	7.740E+00	20	G006	1 2 1 1 1	
6.067E-02	7.050E+00	20.2	S307	1 1 0 2 2	
1.935E-01	2.248E+01	24.50	O005	2 0 2 2 1	
5.982E-02	6.951E+00	25	G006	1 2 1 1 1	
5.727E-02	6.655E+00	30	G006	1 2 1 1 1	
5.489E-02	6.379E+00	30.6	S307	1 1 0 2 2	
4.562E-02	5.302E+00	39.5	S307	1 1 0 2 2	
4.332E-02	5.035E+00	49.7	S307	1 1 0 2 2	
3.992E-02	4.638E+00	60.3	S307	1 1 0 2 2	
3.778E-02	4.391E+00	70.2	S307	1 1 0 2 2	
3.667E-02	4.262E+00	80.2	S307	1 1 0 2 2	
3.855E-02	4.480E+00	90.6	S307	1 1 0 2 2	

1312. $C_7H_{16}O$

2,4-Dimethyl-2-pentanol
2,4-Dimethylpentanol-2
RN: 625-06-9 **MP** (°C)**:** <–20
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-01	1.478E+01	20	G006	1 2 1 1 2	
1.138E-01	1.322E+01	25	G006	1 2 1 1 2	
1.037E-01	1.205E+01	30	G006	1 2 1 1 2	

1313. $C_7H_{16}O$

2,3-Dimethyl-2-pentanol
2,3-Dimethylpentanol-2
RN: 4911-70-0 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-01	1.662E+01	20	G006	1 2 1 1 2	
1.305E-01	1.517E+01	25	G006	1 2 1 1 2	
1.188E-01	1.381E+01	30	G006	1 2 1 1 2	

1314. $C_7H_{16}O$

2,3,3-Trimethyl-2-butanol
Dimethyl-*tert*-butylcarbinol
1,1,2,2-Tetramethylpropanol
1,1,2,2-Tetramethylpropyl alcohol
RN: 594-83-2 **MP** (°C)**:** 17
MW: 116.20 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.852E-01	2.153E+01	40	G006	1 2 1 1 2	

1315. $C_7H_{16}O$

2,2-Dimethyl-3-pentanol
2,2-Dimethylpentanol-3
RN: 3970-62-5 **MP** (°C)**:** –5
MW: 116.20 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.507E-02	8.723E+00	20	G006	1 2 1 1 1	
6.999E-02	8.133E+00	25	G006	1 2 1 1 1	
6.745E-02	7.838E+00	30	G006	1 2 1 1 1	

1316. $C_7H_{16}O$

1-Heptanol
1-Hydroxyheptane
Heptan-1-ol
Heptanol-(1)
n-Heptyl alcohol
RN: 111-70-6 **MP** (°C)**:** –34.6
MW: 116.20 **BP** (°C)**:** 175.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.916E-02	3.388E+00	0	E029	1 2 0 1 1	
2.026E-02	2.354E+00	0	S307	1 1 0 2 2	
1.897E-02	2.205E+00	6.04	H110	2 2 2 2 2	

(*continued*)

1316. $C_7H_{16}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-02	2.593E+00	10	E029	1 2 0 1 1	
1.739E-02	2.020E+00	10.24	H110	2 2 2 2 2	
2.172E-02	2.524E+00	10.5	S307	1 1 0 2 2	
1.720E-02	1.999E+00	10.54	H110	2 2 2 2 2	
1.067E-02	1.240E+00	11.4	N042	1 0 2 1 1	
1.608E-02	1.869E+00	15.04	H110	2 2 2 2 2	
1.544E-02	1.795E+00	17.94	H110	2 2 2 2 2	
8.000E-03	9.296E-01	18	F001	1 0 1 0 2	
8.605E-03	1.000E+00	18	F300	1 0 0 0 1	
1.478E-02	1.717E+00	20	A015	1 2 1 1 2	
1.718E-02	1.996E+00	20	E029	1 2 0 1 1	
1.450E-02	1.685E+00	20	H330	0 0 0 0 0	
1.507E-02	1.751E+00	20.04	H110	2 2 2 2 2	
1.581E-02	1.837E+00	20.2	S307	1 1 0 2 2	
1.476E-02	1.716E+00	21.94	H110	2 2 2 2 2	
1.450E-02	1.685E+00	23.94	H110	2 2 2 2 2	
1.443E-02	1.677E+00	24.94	H110	2 2 2 2 2	
1.546E-02	1.797E+00	25	B038	1 2 1 1 2	
1.000E+00	1.162E+02	25	F044	1 0 0 0 0	EFG
1.460E-02	1.697E+00	25	K025	2 1 1 1 1	
1.434E-02	1.666E+00	25.04	H110	2 2 2 2 2	
1.423E-02	1.653E+00	26.04	H110	2 2 2 2 2	
1.411E-02	1.640E+00	28.04	H110	2 2 2 2 2	
1.375E-02	1.597E+00	30	E029	1 2 0 1 1	
1.397E-02	1.624E+00	30.14	H110	2 2 2 2 2	
1.399E-02	1.626E+00	30.14	H110	2 2 2 2 2	
1.323E-02	1.538E+00	30.6	S307	1 1 0 2 2	
1.386E-02	1.611E+00	32.94	H110	2 2 2 2 2	
1.426E-02	1.657E+00	39.8	S307	1 1 0 2 2	
1.117E-02	1.298E+00	40	E029	1 2 0 1 1	
9.456E-03	1.099E+00	50	E029	1 2 0 1 1	
1.392E-02	1.617E+00	50.1	S307	1 1 0 2 2	
9.456E-03	1.099E+00	60	E029	1 2 0 1 1	
1.529E-02	1.777E+00	60.0	S307	1 1 0 2 2	
1.289E-02	1.498E+00	70	E029	1 2 0 1 1	
1.080E-02	1.255E+00	70	F001	1 0 1 0 2	
1.752E-02	2.036E+00	70.1	S307	1 1 0 2 2	
1.632E-02	1.896E+00	80	E029	1 2 0 1 1	
1.460E-02	1.697E+00	80	F001	1 0 1 0 2	
1.863E-02	2.165E+00	80.1	S307	1 1 0 2 2	
1.975E-02	2.295E+00	90	E029	1 2 0 1 1	
1.940E-02	2.254E+00	90	F001	1 0 1 0 2	
2.086E-02	2.424E+00	90.5	S307	1 1 0 2 2	
2.488E-02	2.892E+00	100	E029	1 2 0 1 1	
2.460E-02	2.859E+00	100	F001	1 0 1 0 2	
2.582E-02	3.000E+00	100	F300	1 0 0 0 1	
3.001E-02	3.488E+00	110	E029	1 2 0 1 1	
3.060E-02	3.556E+00	110	F001	1 0 1 0 2	
3.685E-02	4.282E+00	120	E029	1 2 0 1 1	

(*continued*)

1316. $C_7H_{16}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.537E-02	5.272E+00	130	E029	1 2 0 1 1	
5.557E-02	6.458E+00	140	E029	1 2 0 1 1	
6.830E-02	7.937E+00	150	E029	1 2 0 1 1	
8.352E-02	9.705E+00	160	E029	1 2 0 1 1	
1.046E-01	1.215E+01	170	E029	1 2 0 1 2	
1.355E-01	1.575E+01	180	E029	1 2 0 1 2	
1.753E-01	2.038E+01	190	E029	1 2 0 1 2	
2.213E-01	2.572E+01	200	E029	1 2 0 1 2	
2.894E-01	3.363E+01	210	E029	1 2 0 1 2	
3.847E-01	4.471E+01	220	E029	1 1 0 1 2	
5.404E-01	6.279E+01	230	E029	1 2 0 1 2	
7.894E-01	9.173E+01	240	E029	1 2 0 1 2	
1.054E+00	1.225E+02	245	E029	1 2 0 1 2	
1.029E-02	1.195E+00	ns	H012	0 2 2 0 2	
1.558E-02	1.810E+00	ns	L003	0 0 2 1 2	

1317. $C_7H_{16}O$

Isopropyl *tert*-butyl ether
2-Methyl-2-(1-methylethoxy)-propane
t-Butyl isopropyl ether

RN: 17348-59-3 **MP** (°C)**:** –88
MW: 116.20 **BP** (°C)**:** 87.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.303E-03	5.000E-01	25	K072	1 0 1 1 1	
4.303E-03	5.000E-01	25	M087	1 1 2 1 1	

1318. $C_7H_{16}O$

Heptanol

RN: 53535-33-4 **MP** (°C)**:** –36
MW: 116.20 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.173E+01	20	S006	1 0 0 0 2	
1.240E-02	1.441E+00	24	H345	0 0 0 0 0	

1319. $C_7H_{16}O$

4-Heptanol
Dipropyl carbinol

RN: 589-55-9 **MP** (°C)**:** –42
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.090E-02	4.753E+00	20	H330	0 0 0 0 0	

1320. $C_7H_{16}O$
2,3-Dimethyl-3-pentanol
2,3-Dimethylpentanol-3
RN: 595-41-5 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	1.836E+01	20	G006	1 2 1 1 2	
1.389E-01	1.614E+01	25	G006	1 2 1 1 2	
1.213E-01	1.410E+01	30	G006	1 2 1 1 2	

1321. $C_7H_{16}O_4S_2$
Sulfonmethane
Sulfonal
RN: 115-24-2 **MP** (°C)**:** 125
MW: 228.33 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.962E-02	1.361E+01	16	A072	1 0 1 0 2	
5.956E-02	1.360E+01	16	F300	1 0 0 0 2	
1.027E-02	2.345E+00	18	F062	1 0 2 2 2	
2.847E-01	6.500E+01	100	F300	1 0 0 0 1	
5.888E-02	1.345E+01	ns	R427	0 0 0 0 0	

1322. $C_7H_{16}O_7$
(+)-Perseitol
D-Manno-α-heptit
RN: 527-06-0 **MP** (°C)**:** 188
MW: 212.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.044E-01	6.460E+01	18	F300	1 0 0 0 2	
1.466E+00	3.110E+02	74	F300	1 0 0 0 1	

1323. $C_7H_{17}O_2PS_3$
Phorate
Thimet
Rampart
Phosphorodithioic acid *O,O*-diethyl *S*-[(ethylthio)methyl] ester
American Cyanamid 3911
CL 35024
RN: 298-02-2 **MP** (°C)**:** –43
MW: 260.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-05	1.790E-02	20	B169	2 1 1 1 1	
1.905E-04	4.961E-02	20	B179	0 0 0 0 0	

(*continued*)

1323. $C_7H_{17}O_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.681E-05	2.000E-02	24	F179	2 2 2 2 2	
2.688E-04	7.000E-02	ns	M061	0 0 0 0 1	
1.920E-04	5.000E-02	rt	M161	0 0 0 0 1	

1324. $C_7H_{17}O_2PS_3$

S-2-Isopropylthioethyl *O,O*-dimethyl phosphorodithioate
Isothioate
O,O-Dimethyls-isopropylthioethyl phosphoroditjioate
RN: 36614-38-7 **MP** (°C)**:**
MW: 260.38 **BP** (°C)**:** 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.725E-04	9.700E-02	25	M161	1 0 0 0 1	
3.725E-04	9.700E-02	25	N304	1 0 0 0 1	

1325. $C_7H_{17}O_4PS_3$

Phorate sulfone
O,O′-Diethyl *S*-ethylsulfonylmethyl-phosphorodithioate
Thimet sulfone
CL 18161
Phosphorodithioic acid *O,O*-diethyl *S*-[(ethylsulfonyl)methyl] ester
RN: 2588-04-7 **MP** (°C)**:**
MW: 292.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E-03	8.593E-01	19	B169	2 0 1 1 2	

1326. $C_8H_2Cl_4N_2$

Chlorquinox
5,6,7,8-Tetrachloroquinoxaline
Lucel
Tetrachloroquinoxaline
RN: 3495-42-9 **MP** (°C)**:** 190
MW: 267.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.732E-06	1.000E-03	25	M161	1 0 0 0 0	

1327. $C_8H_2Cl_4O_4$
Tetrachlorophthalic acid
Tetrachlorphthalsaeure
Tetrachloro-1,2-benzenedicarboxylic acid
RN: 632-58-6 **MP** (°C)**:**
MW: 303.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-02	5.700E+00	14	F300	1 0 0 0 1	
1.007E-01	3.060E+01	99	F300	1 0 0 0 2	

1328. $C_8H_3Cl_2F_3N_2$
Chlorflurazole
4,5-Dichloro-2-(trifluoromethyl)-benzimidazole
Dichloro-2-(trifluoromethyl)benzimidazole
2-Trifluoromethyl-4,5-dichlorobenzimidazole
RN: 3615-21-2 **MP** (°C)**:**
MW: 255.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-04	6.000E-02	ns	B100	0 0 0 0 0	
2.353E-04	6.000E-02	ns	M061	0 0 0 0 1	

1329. $C_8H_3Cl_5O_2$
Pentachlorophenyl acetate
Pentachlorophenol acetate
Rabcon
RN: 1441-02-7 **MP** (°C)**:**
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-05	2.000E-02	ns	L311	0 0 0 0 1	

1330. $C_8H_3Cl_5O_3$
2,3,4,5,6-Pentachlorophenoxyacetic acid
Pentachlorophenoxyacetic acid
RN: 2877-14-7 **MP** (°C)**:**
MW: 324.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	5.839E-02	25	L030	1 0 2 1 1	

1331. $C_8H_4Cl_4O_3$
2,3,4,6-Tetrachlorophenoxyacetic acid
Acetic acid, (2,3,4,6-tetrachlorophenoxy)-
RN: 10587-37-8 **MP** (°C)**:**
MW: 289.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.131E-01	25	L030	1 0 2 1 1	

1332. $C_8H_4N_2$
1,4-Benzenedicarbonitrile
Terephthalonitrile
1,4-Dicyanobenzene
RN: 623-26-7 **MP** (°C)**:**
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.970E-04	8.931E-02	25	C316	0 0 0 0 0	0.1M NaCl

1333. $C_8H_4N_2S$
m-Cyanophenyl isothiocyanate
3-Isothiocyanato-benzonitrile
3-Cyanophenyl isothiocyanate
RN: 3125-78-8 **MP** (°C)**:**
MW: 160.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.410E-04	1.027E-01	25	K032	2 2 0 1 2	

1334. $C_8H_4N_2S_2$
m-Isothiocyanophenyl isothiocyanate
3-Isothiocyanophenyl isothiocyanate
RN: 3125-77-7 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.845E-03	25	K032	2 2 0 1 1	

1335. $C_8H_4O_3$
Phthalic anhydride
1,2-Benzenedicarboxylic acid anhydride
1,3-Isobenzofurandione
Phthalic acid anhydride
1,3-Dioxophthalan
1,3 Phthalandione
RN: 85-44-9 **MP** (°C)**:** 130.8
MW: 148.12 **BP** (°C)**:** 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-02	6.200E+00	26.70	L095	2 2 1 1 2	
4.027E-02	5.964E+00	rt	D021	0 0 1 1 2	

1336. $C_8H_5ClO_4$
3-Chlorophthalic acid
3-Chlor-phthalsaeure
RN: 27563-65-1 **MP** (°C)**:**
MW: 200.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-01	2.120E+01	14	F300	1 0 0 0 2	

1337. $C_8H_5Cl_3O_2$
Chlorfenac
2,3,6-Trichlorophenylacetic acid
Fenac
RN: 85-34-7 **MP** (°C)**:** 161
MW: 239.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.351E-04	2.000E-01	28	M161	1 0 0 0 2	
8.351E-04	2.000E-01	30	M061	1 0 0 0 2	

1338. $C_8H_5Cl_3O_3$
2,4,5-Trichlorophenoxyacetic acid
Acetic acid, (2,4,5-trichlorophenoxy)-
(2,4,5-Trichlorophenoxy)acetic acid
2,4,5-T
RN: 93-76-5 **MP** (°C)**:** 156
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.316E-04	2.380E-01	20	B185	0 0 0 0 0	
7.398E-04	1.890E-01	20	M061	1 0 0 0 2	
1.090E-03	2.785E-01	24.99	N417	0 0 0 0 0	

(*continued*)

1338. $C_8H_5Cl_3O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.810E-01	25	B164	1 0 1 1 2	
1.096E-03	2.800E-01	25	B185	0 0 0 0 0	
1.050E-03	2.683E-01	25	L030	1 0 2 1 2	
1.088E-03	2.780E-01	25	M161	1 0 0 0 2	
9.316E-04	2.380E-01	30	B200	1 0 0 0 2	
9.783E-04	2.499E-01	ns	B100	0 0 0 0 1	
7.828E-04	2.000E-01	ns	B185	0 0 0 0 0	
8.000E-04	2.044E-01	ns	F184	0 0 0 0 1	
9.316E-04	2.380E-01	ns	K138	0 0 0 0 1	
9.824E-04	2.510E-01	ns	L024	0 0 0 0 2	
2.512E-04	6.418E-02	ns	M163	0 0 0 0 0	EFG
7.828E-04	2.000E-01	ns	N013	0 0 0 0 2	

1339. $C_8H_5Cl_3O_3$
3,4,5-Trichlorophenoxyacetic acid
Acetic acid, (3,4,5-trichlorophenoxy)-
3,4,5-T
RN: 80496-87-3 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	2.938E-01	25	L030	1 0 2 1 2	

1340. $C_8H_5Cl_3O_3$
2,3,4-Trichlorophenoxyacetic acid
Acetic acid, (2,3,4-trichlorophenoxy)-
2,3,4-T
RN: 25141-27-9 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	2.044E-01	25	L030	1 0 2 1 1	

1341. $C_8H_5Cl_3O_3$
2,4,6-Trichlorophenoxyacetic acid
Acetic acid, (2,4,6-trichlorophenoxy)-
2,4,6-T
RN: 575-89-3 **MP** (°C)**:** 45
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	2.478E-01	25	L030	1 0 2 1 1	

1342. $C_8H_5Cl_3O_3$
2,3,6-Trichlorophenoxyacetic acid
Acetic acid, (2,3,6-trichlorophenoxy)-
2,3,6-T
RN: 4007-00-5 **MP** (°C)**:** 148
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	6.132E-01	25	L030	1 0 2 1 2	

1343. $C_8H_5Cl_3O_3$
2,3,5-Trichlorophenoxyacetic acid
Acetic acid, (2,3,5-trichlorophenoxy)-
2,3,5-T
RN: 33433-95-3 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.555E-01	25	L030	1 0 2 1 2	

1344. $C_8H_5F_3O$
2,2,2-Trifluoroacetophenone
Trifluoroacetophenone
α,α,α-Trifluoroacetophenone
Phenyl trifluoromethyl ketone
2,2,2-Trifluoro-1-phenylethanone
RN: 434-45-7 **MP** (°C)**:** –40
MW: 174.12 **BP** (°C)**:** 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.007E-02	1.220E+01	30	B433	0 0 0 0 0	

1345. $C_8H_5F_3O_2$
α,α,α-Trifluoro-*o*-toluic acid
Trifluoro-*o*-toluic acid
Acide orthotrifluortoluique
RN: 433-97-6 **MP** (°C)**:** 111
MW: 190.12 **BP** (°C)**:** 247

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	4.800E+00	25	D064	1 2 1 1 2	

1346. $C_8H_5NO_2$
Phthalimide
Phthalimid
RN: 85-41-6 **MP** (°C)**:** 238.0
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.447E-03	3.600E-01	25	F300	1 0 0 0 1	
2.719E-02	4.000E+00	100	F300	1 0 0 0 0	
4.075E-03	5.996E-01	rt	D021	0 0 1 1 0	

1347. $C_8H_5NO_2S$
3-Carboxyphenylisothiocyanate
m-Isothiocyanobenzoic acid
RN: 2131-63-7 **MP** (°C)**:**
MW: 179.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-04	1.004E-01	25	D019	1 1 1 1 2	
8.000E-04	1.434E-01	25	K032	2 2 0 1 1	

1348. $C_8H_5NO_2S$
4-Carboxyphenylisothiocyanate
p-Carboxyphenylisothiocyanate
RN: 2131-62-6 **MP** (°C)**:**
MW: 179.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	1.900E-02	25	D019	1 1 1 1 2	

1349. $C_8H_5NO_4$
6-Nitrophthalide
6-Nitro-phthalid
RN: 610-93-5 **MP** (°C)**:** 145
MW: 179.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-03	4.000E-01	25	F300	1 0 0 0 2	

1350. $C_8H_5NO_6$
3-Nitrophthalic acid
3-Nitro-phthalsaeure
RN: 603-11-2 **MP** (°C)**:** 218
MW: 211.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.520E-02	2.010E+01	25	F300	1 0 0 0 2	

1351. $C_8H_5NO_6$
2,3,4-Pyridinetricarboxylic acid
Pyridin-tricarbonsaeure-(2,3,4)
RN: 632-95-1 **MP** (°C)**:** 250
MW: 211.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.684E-02	1.200E+01	15	F300	1 0 0 0 1	

1352. C_8H_6
Ethynylbenzene
Phenylacetylene
RN: 536-74-3 **MP** (°C)**:** –44.8
MW: 102.14 **BP** (°C)**:** 142.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.467E-03	4.562E-01	ns	D001	0 0 0 0 2	

1353. C_8H_6BrNS
3-Bromobenzyl isothiocyanate
m-Bromobenzyl isothiocyanate
RN: 3845-33-8 **MP** (°C)**:**
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.441E-02	25	D014	1 0 0 0 1	

1354. C_8H_6BrNS
4-Bromobenzyl isothiocyanate
p-Bromobenzyl isothiocyanate
RN: 2076-56-4 **MP** (°C)**:**
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.483E-02	25	D014	1 0 0 0 1	
1.500E-04	3.422E-02	25	D019	1 1 1 1 2	

1355. C_8H_6ClNS
3-Chlorobenzyl isothiocyanate
m-Chlorobenzyl isothiocyanate
RN: 3694-58-4 **MP** (°C)**:**
MW: 183.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	2.516E-02	25	D014	1 0 0 0 1	

1356. C_8H_6ClNS
4-Chlorobenzyl isothiocyanate
p-Chlorobenzyl isothiocyanate
RN: 3694-45-9 **MP** (°C)**:**
MW: 183.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	2.718E-02	25	D014	1 0 0 0 1	

1357. $C_8H_6Cl_2O_3$
2,4-Dichlorophenoxyacetic acid
2,4-D
(2,4-Dichlorophenoxy)acetic acid
RN: 94-75-7 **MP** (°C)**:** 138
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.805E-03	6.200E-01	20	F311	1 2 2 2 1	
2.443E-03	5.400E-01	20	M061	1 0 0 0 2	
2.939E-03	6.496E-01	21.50	B200	1 0 0 0 0	
4.072E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.060E-03	6.764E-01	24.99	N417	0 0 0 0 0	
3.085E-03	6.820E-01	25	B164	1 0 1 1 2	
3.280E-03	7.250E-01	25	B185	0 0 0 0 0	
4.026E-03	8.900E-01	25	F071	1 1 2 1 2	
2.360E-03	5.217E-01	25	L030	1 0 2 1 2	
2.805E-03	6.200E-01	25	M161	1 0 0 0 2	
2.713E-03	5.996E-01	ns	B100	0 0 0 0 0	
4.072E-03	9.000E-01	ns	B185	0 0 0 0 0	
1.810E-03	4.000E-01	ns	B185	0 0 0 0 0	
2.500E-03	5.526E-01	ns	F184	0 0 0 0 1	
4.072E-03	9.000E-01	ns	K138	0 0 0 0 1	
2.805E-03	6.200E-01	ns	L024	0 0 0 0 2	
4.298E-03	9.500E-01	ns	M110	0 0 0 0 0	EFG
1.259E-03	2.783E-01	ns	M163	0 0 0 0 0	EFG
4.026E-03	8.900E-01	ns	M344	0 0 0 0 2	
2.488E-03	5.500E-01	ns	N013	0 0 0 0 2	

1358. $C_8H_6Cl_2O_3$
Dicamba
2-Methoxy-3,6-dichlorobenzoic acid
RN: 1918-00-9 **MP** (°C)**:** 98
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.036E-02	4.500E+00	25	B200	1 0 0 0 1	
2.036E-02	4.500E+00	25	M161	1 0 0 0 1	
3.591E-02	7.937E+00	ns	B100	0 0 0 0 0	

1359. $C_8H_6Cl_2O_3$
3,5-Dichlorophenoxyacetic acid
3,5-D
RN: 587-64-4 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-03	9.615E-01	25	L030	1 0 2 1 2	

1360. $C_8H_6Cl_2O_3$
3,4-Dichlorophenoxyacetic acid
3,4-D
RN: 588-22-7 **MP** (°C)**:** 138
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-03	4.576E-01	25	L030	1 0 2 1 2	
2.090E-03	4.620E-01	ns	B185	0 0 0 0 0	

1361. $C_8H_6Cl_2O_3$
2,6-Dichlorophenoxyacetic acid
2,6-D
RN: 575-90-6 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-03	1.558E+00	25	L030	1 0 2 1 2	

1362. $C_8H_6Cl_2O_3$
2,3-Dichlorophenoxyacetic acid
2,3-D
RN: 2976-74-1 **MP** (°C)**:** 173
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-03	3.426E-01	25	L030	1 0 2 1 2	

1363. $C_8H_6Cl_2O_3$
2,5-Dichlorophenoxyacetic acid
2,5-D
RN: 582-54-7 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-03	5.349E-01	25	L030	1 0 2 1 2	

1364. $C_8H_6Cl_4O_2$
Tetrachloroveratrole
3,4,5,6-Tetrachloro-1,2-dimethoxybenzene
RN: 944-61-6 **MP** (°C)**:**
MW: 275.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.762E-06	1.590E-03	25	L348	1 2 2 1 2	

1365. $C_8H_6Cl_5NO_2$
Penclomedine
Pyridine
3,5-Dichloro-2,4-dimethoxy-6-(trichloromethyl)
NSC 338720
RN: 108030-77-9 **MP** (°C)**:**
MW: 325.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.229E-06	4.000E-04	25	P325	0 0 0 0 0	
1.229E-06	4.000E-04	25	P336	0 0 0 0 0	

1366. $C_8H_6F_3N_3O_4S_2$
Flumethiazide
6-(Trifluoromethyl)-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
6-Trifluoromethyl-7-sulfamoyl-4H-1,2,4-benzothiadiazine 1,1-dioxide
Trifluoromethylthiazide
RN: 148-56-1 **MP** (°C)**:**
MW: 329.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.189E-03	1.050E+00	rt	A095	0 0 2 2 2	

1367. C_8H_6INS
3-Iodobenzyl isothiocyanate
m-Iodobenzyl isothiocyanate
RN: 3696-68-2 **MP** (°C)**:**
MW: 275.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	1.513E-02	25	D014	1 0 0 0 1	

1368. C_8H_6INS
4-Iodobenzyl isothiocyanate
p-Iodobenzyl isothiocyanate
RN: 3694-49-3 **MP** (°C)**:**
MW: 275.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-05	1.403E-02	25	D014	1 0 0 0 1	

1369. $C_8H_6N_2O_2S$
3-Nitrobenzyl isothiocyanate
m-Nitrobenzyl isothiocyanate
RN: 3696-69-3 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.593E-02	25	D014	1 0 0 0 1	

1370. $C_8H_6N_2O_2S$
4-Nitrobenzyl isothiocyanate
p-Nitrobenzyl isothiocyanate
RN: 3694-47-1 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	4.525E-02	25	D014	1 0 0 0 1	

1371. $C_8H_6N_4O_5$
Nitrofurantoin
1-[(5-Nitrofurfurylidene)amino]hydantoin
Furatoin
Macrodantin
Macrobid
Welfurin
RN: 67-20-9 **MP** (°C)**:** 268
MW: 238.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.619E-04	1.100E-01	22	B154	1 1 1 1 1	pH 3.5
3.338E-04	7.950E-02	24	C034	2 0 2 2 2	
3.338E-04	7.950E-02	24	C118	1 0 0 0 2	
5.207E-04	1.240E-01	25	M457	0 0 0 0 0	
4.753E-04	1.132E-01	30	C011	2 0 2 1 0	EFG
4.761E-04	1.134E-01	30	C034	2 0 2 2 2	
4.761E-04	1.134E-01	30	C118	1 0 0 0 2	
8.264E-04	1.968E-01	37	A330	0 0 0 0 0	
1.142E-03	2.720E-01	37	B044	2 2 2 1 2	pH 7.2
7.310E-04	1.741E-01	37	C011	2 0 2 1 0	EFG
7.310E-04	1.741E-01	37	C034	2 0 2 2 2	
7.310E-04	1.741E-01	37	C118	1 0 0 0 2	
5.878E-04	1.400E-01	37	E044	1 0 1 1 2	
6.508E-04	1.550E-01	37	P034	1 0 0 0 2	pH 5
1.055E-03	2.512E-01	45	C034	2 0 2 2 2	
1.055E-03	2.512E-01	45	C118	1 0 0 0 2	
7.978E-04	1.900E-01	ns	K444	0 0 0 0 0	
5.249E-04	1.250E-01	ns	P033	0 0 0 0 2	
5.248E-04	1.250E-01	ns	R427	0 0 0 0 0	

1372. $C_8H_6N_4O_8$
Alloxantin
Uroxine
Alloxantin hydrate
RN: 76-24-4 **MP** (°C)**:** 254dec
MW: 286.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-03	5.017E-01	25	B119	1 0 2 2 0	EFG
1.013E-02	2.900E+00	25	F300	1 0 0 0 1	
2.097E-01	6.000E+01	100	F300	1 0 0 0 0	

1373. $C_8H_6N_4S_2$
Methylthiobenzothiazole
Benzothiazole
RN: 76006-86-5 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-04	1.100E-01	22	P323	0 0 0 0 0	

1374. $C_8H_6O_2$
Phthalic dicarboxaldehyde
o-Phthalaldehyd
RN: 643-79-8 **MP** (°C)**:** 56.5
MW: 134.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-01	1.400E+01	h	F300	0 0 0 0 1	

1375. $C_8H_6O_2$
Terephthaldicarboxaldehyde
Terephthalaldehyd
RN: 623-27-8 **MP** (°C)**:** 115
MW: 134.14 **BP** (°C)**:** 246.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	2.000E-01	20	F300	1 0 0 0 0	
1.297E-01	1.740E+01	100	F300	1 0 0 0 1	

1376. $C_8H_6O_3$
Piperonal
Heliotropine
3,4-Dihydroxybenzaldehyde methylene ketal
Methylenedioxy procatechuic aldehyde
Protocatechuic aldehyde methylene ether
Piperonyl aldehyde
RN: 120-57-0 **MP** (°C)**:** 37
MW: 150.14 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-02	3.500E+00	20	F300	1 0 0 0 1	
4.463E-02	6.700E+00	78	F300	1 0 0 0 1	

1377. $C_8H_6O_3$

Benzoylformic acid
Phenyglyoxilic acid
RN: 611-73-4 **MP** (°C)**:** 67
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.128E+00	9.200E+02	0	C020	1 2 1 1 1	

1378. $C_8H_6O_4$

1,4-Benzenedicarboxylic acid
Terephthalic acid
p-Phthalic acid
RN: 100-21-0 **MP** (°C)**:**
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.029E-05	1.500E-02	20	F300	1 0 0 0 1	
1.920E-03	3.190E-01	25	C316	0 0 0 0 0	0.1M HCL
6.019E-04	9.999E-02	80	A027	1 0 0 0 0	

1379. $C_8H_6O_4$

1,2-Benzenedicarboxylic acid
o-Phthalic acid
Phthalic acid
Phthalsaeure
Benzene-1,2-dicarboxylic acid
RN: 88-99-3 **MP** (°C)**:** 230
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.295E+00	0	M043	1 0 0 0 1	
2.219E-02	3.686E+00	2	A027	1 0 0 0 1	
2.159E-02	3.587E+00	10	M043	1 0 0 0 1	
7.935E-03	1.318E+00	10	S198	2 1 2 2 2	
1.571E-02	2.611E+00	10.49	A341	0 0 0 0 0	
3.471E-02	5.767E+00	20	A027	1 0 0 0 1	
3.435E-02	5.707E+00	20	F069	2 2 2 2 2	
3.431E-02	5.700E+00	20	F300	1 0 0 0 1	
3.352E-02	5.569E+00	20	M043	1 0 0 0 1	
7.214E-03	1.199E+00	20	S198	2 1 2 2 2	
3.915E-02	6.504E+00	22.99	A341	0 0 0 0 0	
4.200E-02	6.978E+00	24.99	A341	0 0 0 0 0	
8.600E-02	1.429E+01	25	H084	1 0 0 0 1	
8.520E-02	1.415E+01	25	K040	1 0 2 1 2	
4.192E-02	6.965E+00	25	M030	2 1 0 1 2	
4.279E-02	7.109E+00	25.8	W029	1 2 1 1 2	
4.808E-02	7.988E+00	28	D050	1 2 1 2 2	
5.152E-02	8.560E+00	29.49	A341	0 0 0 0 0	

(*continued*)

1379. $C_8H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	8.141E+00	30	H019	0 0 0 0 0	
4.777E-02	7.937E+00	30	M043	1 0 0 0 0	
8.235E-03	1.368E+00	30	S198	2 1 2 2 2	
5.865E-02	9.743E+00	33.99	A341	0 0 0 0 0	
6.033E-02	1.002E+01	35	M030	2 1 0 1 2	
6.561E-02	1.090E+01	35.99	A341	0 0 0 0 0	
6.925E-02	1.150E+01	37.99	A341	0 0 0 0 0	
7.137E-02	1.186E+01	40	M043	1 0 0 0 1	
8.274E-02	1.375E+01	41.99	A341	0 0 0 0 0	
7.865E-02	1.307E+01	43.7	W029	1 2 1 1 2	
8.981E-02	1.492E+01	43.99	A341	0 0 0 0 0	
8.991E-02	1.494E+01	44.99	A341	0 0 0 0 0	
8.580E-02	1.425E+01	45	M030	2 1 0 1 2	
9.890E-02	1.643E+01	45.99	A341	0 0 0 0 0	
9.753E-02	1.620E+01	48.9	W029	1 2 1 1 2	
1.212E-01	2.014E+01	49.99	A341	0 0 0 0 0	
1.116E-01	1.854E+01	49.99	A341	0 0 0 0 0	
1.349E-01	2.241E+01	53.99	A341	0 0 0 0 0	
1.277E-01	2.122E+01	55	M030	2 1 0 1 2	
1.339E-01	2.225E+01	58.0	W029	1 2 1 1 2	
1.639E-01	2.724E+01	60	M043	1 0 0 0 1	
1.741E-01	2.892E+01	60.99	A341	0 0 0 0 0	
1.695E-01	2.815E+01	63.7	W029	1 2 1 1 2	
2.145E-01	3.564E+01	64.99	A341	0 0 0 0 0	
1.892E-01	3.144E+01	65	M030	2 1 0 1 2	
2.826E-01	4.695E+01	75	M030	2 1 0 1 2	
3.042E-01	5.053E+01	77.8	W029	1 2 1 1 2	
3.567E-01	5.927E+01	80	M043	1 0 0 0 1	
4.334E-01	7.200E+01	85	F300	1 0 0 0 0	
4.297E-01	7.138E+01	85	M030	2 1 0 1 2	
4.248E-01	7.058E+01	85.7	W029	1 2 1 1 2	
6.377E-01	1.059E+02	94.8	W029	1 2 1 1 2	
9.182E-01	1.525E+02	100	M043	1 0 0 0 2	
8.208E-01	1.364E+02	101.1	W029	1 2 1 1 2	
1.370E+00	2.276E+02	113.8	W029	1 2 1 1 2	
9.015E-03	1.498E+00	ns	F014	0 0 0 0 2	
2.458E-02	4.083E+00	rt	H431	0 0 0 0 0	

1380. $C_8H_6O_4$

Isophthalic acid
1,3-Benzenedicarboxylic acid
m-Phthalic acid

RN: 121-91-5 **MP** (°C)**:** 345
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.611E-04	6.000E-02	2	A027	1 0 0 0 0	
6.019E-04	9.999E-02	20	A027	1 0 0 0 0	

(*continued*)

1380. $C_8H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-03	1.811E-01	28.29	L437	0 0 0 0 0	
1.656E-03	2.752E-01	40.99	L437	0 0 0 0 0	
2.535E-03	4.212E-01	51.99	L437	0 0 0 0 0	
4.021E-03	6.681E-01	64.99	L437	0 0 0 0 0	
6.260E-03	1.040E+00	76.49	L437	0 0 0 0 0	
6.013E-03	9.990E-01	80	A027	1 0 0 0 0	
8.300E-03	1.379E+00	83.49	L437	0 0 0 0 0	
9.441E-03	1.568E+00	86.47	L437	0 0 0 0 0	
1.286E-02	2.137E+00	93.42	L437	0 0 0 0 0	
4.610E-04	7.659E-02	rt	H431	0 0 0 0 0	

1381. $C_8H_6O_5$

2-Hydroxyisophthalic acid
2-Hydroxy-*iso*-phthalsaeure

RN: 606-19-9 **MP** (°C)**:** 244
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-01	2.640E+01	100	F300	1 0 0 0 2	

1382. $C_8H_6O_5$

4-Hydroxyisophthalic acid
4-Hydroxy-*iso*-phthasaeure

RN: 636-46-4 **MP** (°C)**:** 310
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.647E-03	3.000E-01	24	F300	1 0 0 0 1	

1383. $C_8H_6O_5$

5-Hydroxyisophthalic acid
5-Hydroxy-*iso*-phthalsaeure

RN: 618-83-7 **MP** (°C)**:** 293
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.294E-03	6.000E-01	15	F300	1 0 0 0 1	
8.889E-01	1.619E+02	99	F300	1 0 0 0 2	

1384. C_8H_6S

Thianaphthene
Benzo[b]thiophene
Benzothiofuran
1-Benzothiophene

RN: 95-15-8 **MP** (°C)**:** 29–32
MW: 134.20 **BP** (°C)**:** 221–222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-03	2.162E-01	59.0	L339	2 0 2 2 2	
2.610E-03	3.503E-01	78.5	L339	2 0 2 2 2	
4.386E-03	5.886E-01	99.0	L339	2 0 2 2 2	

1385. $C_8H_7BrN_2O_3$

o-Nitro-*o*-bromacetanilide
2-Bromo-5-nitroacetanilide

RN: 245115-83-7 **MP** (°C)**:**
MW: 259.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.720E-02	2.000E+01	rt	F043	0 0 2 1 1	

1386. $C_8H_7BrN_2O_3$

p-Nitro-*o*-bromacetanilide
2-Bromo-4-nitroacetanilide

RN: 57045-86-0 **MP** (°C)**:**
MW: 259.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.832E-02	1.770E+01	rt	F043	0 0 2 1 2	

1387. $C_8H_7ClN_2O_3$

p-Nitro-*o*-chloracetanilide
2-Chloro-4-nitroacetanilide

RN: 881-87-8 **MP** (°C)**:**
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1388. $C_8H_7ClN_2O_3$
o-Nitro-*o*-chloracetanilide
2-Chloro-5-nitroacetanilide
RN: 72487-80-0 **MP** (°C)**:**
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1389. $C_8H_7ClO_3$
4-Chlorophenoxyacetic acid
4-CPA
p-Chlorophenoxyacetic acid
RN: 122-88-3 **MP** (°C)**:** 157
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.545E-03	8.480E-01	25	B164	1 0 1 1 2	
2.042E-03	3.810E-01	25	B185	0 0 0 0 0	
5.130E-03	9.572E-01	25	L030	1 0 2 1 2	

1390. $C_8H_7ClO_3$
3-Chlorophenoxyacetic acid
m-Chlorophenoxyacetic acid
RN: 588-32-9 **MP** (°C)**:**
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E-02	2.360E+00	25	L030	1 0 2 1 2	

1391. $C_8H_7ClO_3$
2-Chlorophenoxyacetic acid
o-Chlorophenoxyacetic acid
RN: 614-61-9 **MP** (°C)**:** 146
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.850E-03	1.278E+00	25	L030	1 0 2 1 2	

1392. $C_8H_7Cl_2NO_2$
Chloramben methyl ester
Vegiben 2E
Methyl 3-amino-2,5-dichlorobenzoate
Amchem 65-81-B
Methyl chloramben
Chloramben methyl
RN: 7286-84-2 **MP** (°C)**:** 63.5
MW: 220.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.453E-04	1.200E-01	20	M161	1 0 0 0 2	

1393. $C_8H_7Cl_3O$
2,4,6-Trichloro-3,5-dimethyl-phenol
3,5-Xylenol, 2,4,6-trichloro-
RN: 6972-47-0 **MP** (°C)**:**
MW: 225.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	4.961E-03	25	B316	0 0 0 0 0	

1394. $C_8H_7Cl_3O_2$
3,4,5-Trichloroveratrole
4,5,6-Trichloroveratrole
RN: 16766-29-3 **MP** (°C)**:** 66
MW: 241.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.265E-05	1.030E-02	25	L348	1 2 2 1 2	

1395. C_8H_7N
Indole
2,3-Benzopyrrole
Benzopyrrole
1-Benzazole
1-Benzol β pyrrol
RN: 120-72-9 **MP** (°C)**:** 52
MW: 117.15 **BP** (°C)**:** 253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.219E-02	1.080E+01	25	K119	1 0 0 0 2	
3.037E-02	3.558E+00	25	P051	2 1 1 2 2	
3.037E-02	3.558E+00	25.00	P007	2 1 2 2 2	

1396. C_8H_7N
p-Toluonitrile
p-Cyanotoluene
p-Methylbenzonitrile
4-Methylbenzenecarbonitrile
RN: 104-85-8 **MP** (°C)**:**
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.523E+00	25	M327	1 0 0 1 2	

1397. C_8H_7NOS
m-Methoxyphenyl isothiocyanate
3-Methoxyphenyl isothiocyanate
RN: 3125-64-2 **MP** (°C)**:**
MW: 165.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	4.461E-02	25	K032	2 2 0 1 2	

1398. C_8H_7NOS
p-Methoxyphenyl isothiocyanate
4-Methoxyphenylisothiocyanate
RN: 2284-20-0 **MP** (°C)**:** 18.0
MW: 165.22 **BP** (°C)**:** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	4.130E-02	25	D019	1 1 1 1 2	

1399. $C_8H_7NO_3$
Oxanilic acid
N-Phenyloxalic acid monoamide
Oxanilsaure
RN: 500-72-1 **MP** (°C)**:** 150
MW: 165.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.990E-02	8.241E+00	25	D058	1 0 1 1 2	

1400. $C_8H_7NO_4$
6-Nitro-3-methylbenzoic acid
2-Nitro-5-methylbenzoic acid
5-Methyl-2-nitrobenzoic acid
3-Methyl-6-nitrobenzoic acid
RN: 3113-72-2 **MP** (°C)**:**
MW: 181.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.043E-02	3.700E+00	10	G063	1 0 0 0 1	
2.595E-02	4.700E+00	20	G063	1 0 0 0 1	
9.385E-02	1.700E+01	40	G063	1 0 0 0 1	
9.937E-02	1.800E+01	50	G063	1 0 0 0 1	
1.490E-01	2.700E+01	60	G063	1 0 0 0 1	
1.932E-01	3.500E+01	65	G063	1 0 0 0 1	
2.484E-01	4.500E+01	70	G063	1 0 0 0 1	
3.643E-01	6.600E+01	80	G063	1 0 0 0 1	
3.699E-01	6.700E+01	100	G063	1 0 0 0 1	

1401. $C_8H_7NO_4$
2-Nitro-3-methylbenzoic acid
2-Nitro-*m*-toluic acid
3-Methyl-2-nitrobenzoic acid
RN: 5437-38-7 **MP** (°C)**:**
MW: 181.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.208E-03	4.000E-01	20	G063	1 0 0 0 1	
8.832E-03	1.600E+00	40	G063	1 0 0 0 1	
3.202E-02	5.800E+00	80	G063	1 0 0 0 1	
3.312E-02	6.000E+00	100	G063	1 0 0 0 0	

1402. C_8H_7NS
Benzyl isothiocyanate
Benzylisothiocyanate
Isothiocyanatomethylbenzene
RN: 622-78-6 **MP** (°C)**:** 112
MW: 149.22 **BP** (°C)**:** 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.089E-01	25	D014	1 0 0 0 2	

1403. C_8H_7NS
p-Tolyl isothiocyanate
4-Tolylisothiocyanate
RN: 622-59-3 **MP** (°C)**:** 25
MW: 149.22 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	2.835E-03	25	D019	1 1 1 1 1	

1404. C_8H_7NS
m-Methylphenyl isothiocyanate
3-Methylphenyl isothiocyanate
RN: 614-69-7 **MP** (°C)**:**
MW: 149.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	2.119E-02	25	K032	2 2 0 1 2	

1405. $C_8H_7N_5O$
7-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.035E-02	7.634E+00	100	A083	1 2 0 0 0	

1406. $C_8H_7N_5O$
2-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	3.226E+01	100	A083	1 2 0 0 0	

1407. $C_8H_7N_5O$
4-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E+00	3.333E+02	100	A083	1 2 0 0 0	

1408. $C_8H_7N_5O_8$
2,4,6-Trinitrophenylethylnitramine
Tetrethyl
Trinitrophenylethylnitramine
Ethyl tetryl
RN: 6052-13-7 **MP** (°C)**:**
MW: 301.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-04	6.000E-02	22	D067	1 2 0 0 0	
8.633E-04	2.600E-01	50	D067	1 2 0 0 1	
8.998E-03	2.710E+00	100	D067	1 2 0 0 2	

1409. C_8H_8
Styrene
Phenylethylene
Styrolene
Styrol
Ethenylbenzene
Annamene
RN: 100-42-5 **MP** (°C)**:** –30
MW: 104.15 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-03	2.899E-01	7	L028	1 0 1 1 1	
2.400E-03	2.499E-01	15	L028	1 0 1 1 1	
1.152E-03	1.200E-01	20	L096	1 2 0 2 2	
3.167E-03	3.299E-01	24	L028	1 0 1 1 1	
2.880E-03	3.000E-01	25	A002	1 2 1 1 1	
1.540E-03	1.604E-01	25	B173	2 0 2 2 2	
2.975E-03	3.099E-01	25	L028	1 0 1 1 1	
3.455E-03	3.599E-01	32	L028	1 0 1 1 1	
3.839E-03	3.998E-01	40	L028	1 0 1 1 1	
3.839E-03	3.998E-01	44	L028	1 0 1 1 1	
4.319E-03	4.498E-01	49	L028	1 0 1 1 1	
4.319E-03	4.498E-01	51	L028	1 0 1 1 1	
4.798E-03	4.998E-01	56	L028	1 0 1 1 1	
8.658E-02	9.018E+00	65	A324	2 2 2 1 1	
5.566E-03	5.797E-01	65	L028	1 0 1 1 1	

1410. $C_8H_8BrCl_2O_3PS$

Bromophos
O-(4-Bromo-2,5-dichlorophenyl) *O,O*-dimethyl phosphorothioate
Nexion
Brofene
Brophene
Omexan

RN: 2104-96-3 **MP** (°C)**:** 51
MW: 366.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.557E-07	2.400E-04	10	B324	0 0 0 0 0	
6.558E-07	2.400E-04	10	B324	0 0 0 0 0	
8.197E-07	3.000E-04	20	B169	2 1 1 1 1	*sic*
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
2.732E-06	1.000E-03	20	F311	1 2 2 2 1	*sic*
1.093E-04	4.000E-02	20	M061	1 0 0 0 1	
1.093E-04	4.000E-02	20	W311	1 0 0 0 1	
2.634E-06	9.641E-04	30	B324	0 0 0 0 0	
2.623E-06	9.600E-04	30	B324	0 0 0 0 0	
1.093E-04	4.000E-02	ns	E050	0 0 0 0 1	
1.093E-04	4.000E-02	rt	M161	0 0 0 0 1	

1411. C_8H_8BrNO

4′-Bromoacetanilide
Acetamide, *N*-(4-bromophenyl)-
Acetanilide, 4′-bromo-
Bromoantifebrin

RN: 103-88-8 **MP** (°C)**:**
MW: 214.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.498E-01	25	D044	0 0 0 0 0	

1412. C_8H_8ClNO

p-Chloroacetanilide
Acetamide, *N*-(4-chlorophenyl)-
Acetanilide, 4′-chloro-

RN: 539-03-7 **MP** (°C)**:**
MW: 169.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.696E-01	25	D044	0 0 0 0 0	

1413. $C_8H_8Cl_2IO_3PS$

Iodofenphos
O-(2,5-Dichloro-4-iodophenyl) *O,O*-dimethyl phosphorothioate
Nuvanol-N
Dimethyl *O*-2,5-dichloro-4-iodophenyl thiophosphate
Alfacron
Jodfenphos

RN: 18181-70-9 **MP** (°C)**:** 72
MW: 413.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.421E-07	1.000E-04	20	B169	2 1 1 1 1	
4.843E-06	2.000E-03	20	M161	1 0 0 0 0	

1414. $C_8H_8Cl_2O$

2,4-Dichloro-6-ethyl-phenol
Phenol, 2,4-dichloro-6-ethyl-

RN: 24539-94-4 **MP** (°C)**:**
MW: 191.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.484E-01	25	B316	0 0 0 0 0	

1415. $C_8H_8Cl_2O_2$

Chloroneb
Demosan
Terraneb
Terraneb SP
1,4-Dichloro-2,5-dimethoxybenzene
Terraneb B

RN: 2675-77-6 **MP** (°C)**:** 134.5
MW: 207.06 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.864E-05	8.000E-03	25	M161	1 0 0 0 0	

1416. $C_8H_8Cl_2O_2$

4,5-Dichloroveratrole
Benzene, 1,2-dichloro-4,5-dimethoxy-

RN: 2772-46-5 **MP** (°C)**:** 83
MW: 207.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-04	7.230E-02	25	L348	1 2 2 1 2	average of 2

1417. $C_8H_8Cl_3O_3PS$

Ronnel
Fenchlorphos
Dermafos
Dimethyl trichlorophenylthiophosphate

RN: 299-84-3 **MP** (°C)**:** 35
MW: 321.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.866E-06	6.000E-04	20	B169	2 2 1 1 1	
3.359E-06	1.080E-03	20	C053	0 0 0 0 0	
3.110E-06	1.000E-03	20	E048	1 2 1 1 0	
7.775E-06	2.500E-03	20	F311	1 2 2 2 1	
5.287E-06	1.700E-03	ns	F040	1 2 2 2 1	
3.359E-06	1.080E-03	ns	F071	0 1 2 1 2	
1.866E-05	6.000E-03	ns	K138	0 0 0 0 1	
1.368E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.244E-04	4.000E-02	rt	M161	0 0 0 0 1	

1418. C_8H_8FNO

4′-Fluoroacetanilide
Acetamide, *N*-(4-fluorophenyl)-
4-Fluoroacetanilide

RN: 351-83-7 **MP** (°C)**:**
MW: 153.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-02	2.496E+00	25	D044	0 0 0 0 0	

1419. $C_8H_8F_3N_3O_4S_2$

Hydroflumethiazide
Diucardin
Saluron

RN: 135-09-1 **MP** (°C)**:** 272
MW: 331.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-03	4.800E-01	37	C087	0 0 0 0 0	
2.048E-03	6.785E-01	37	C315	0 0 0 0 0	0.1N HCL, average of 4
5.643E-04	1.870E-01	ns	B404	0 2 1 1 0	
9.958E-04	3.299E-01	rt	K144	0 0 0 0 1	

1420. C_8H_8INO
p-Iodoaniline-*N*-acetate
4-Iodanilin-*N*-acetat
4-Iodoacetanilide
Acetanilide, 4′-iodo-
4-Acetamidophenyl iodide
p-Iodoacetanilide
RN: 622-50-4 **MP** (°C)**:**
MW: 261.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.827E-01	25	D044	0 0 0 0 0	

1421. $C_8H_8N_2O_2$
Phthalamide
1,2-Benzenedicarboxamide
RN: 88-96-0 **MP** (°C)**:** 228
MW: 164.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-03	2.000E-01	20	A027	1 0 0 0 0	*sic*
3.594E-02	5.900E+00	30	K004	1 0 0 0 1	

1422. $C_8H_8N_2O_2$
Ricinine
Ricinin
RN: 524-40-3 **MP** (°C)**:** 201.5
MW: 164.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-02	2.700E+00	10	F300	1 0 0 0 1	

1423. $C_8H_8N_2O_3$
4-Nitroaniline-*N*-acetate
4-Nitro-anilin-*N*-acetat
p-Nitroacetanilide
1-Nitro-4-acetylaminobenzene
RN: 104-04-1 **MP** (°C)**:** 216
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
6.000E-04	1.081E-01	25	D044	0 0 0 0 0	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1424. $C_8H_8N_2O_3$
2-Nitroaniline-*N*-acetate
2-Nitro-anilin-*N*-acetat
o-Nitroacetanilide
RN: 552-32-9 **MP** (°C)**:**
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1425. $C_8H_8N_2O_6S$
MB 8882
Methyl *N*-(4-nitrobenzenesulphonyl)carbamate
RN: 3337-70-0 **MP** (°C)**:** 151
MW: 260.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.839E-03	9.990E-01	ns	M061	0 0 0 0 0	

1426. $C_8H_8N_4$
6,7-Dimethylpteridine
6:7-Dimethylpteridine
RN: 704-61-0 **MP** (°C)**:**
MW: 160.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-01	5.556E+01	20	A083	1 2 0 0 0	

1427. $C_8H_8N_4$
Hydralazine
Apresoline
RN: 86-54-4 **MP** (°C)**:** 172
MW: 160.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.996E-05	4.800E-03	22.5	B440	0 0 0 0 0	

1428. $C_8H_8N_4O$
4-Hydroxy-6,7-dimethylpteridine
4-Hydroxy-6:7-dimethylpteridine
RN: 14684-54-9 **MP** (°C)**:**
MW: 176.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.155E-03	9.083E-01	22.5	A085	1 2 0 0 0	

1429. $C_8H_8N_4O_2$
H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-oxopropyl)-
RN: 96448-61-2 **MP** (°C)**:**
MW: 192.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	3.000E-01	22	B428	1 2 1 2 1	

1430. $C_8H_8N_4O_2S_2$
2-Sulfanilamido-1,3,4-thiadiazole
Sulfathiadiazole
Sulfanilamide, *N*1-1,3,4-thiadiazol-2-yl-
RN: 16806-29-4 **MP** (°C)**:**
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.848E-03	7.300E-01	37	R045	1 2 1 1 1	

1431. $C_8H_8N_4O_3$
1-Acetoxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(acetyloxy)methyl]-1,5-dihydro-
RN: 98846-64-1 **MP** (°C)**:** 257-258
MW: 208.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	5.800E-01	22	B322	0 0 0 0 0	

1432. $C_8H_8N_4O_4$
Nifuradene
1-[5-Nitrofurfuryllidene)amino]-2-imidazolidinone
RN: 555-84-0 **MP** (°C)**:** 261.5
MW: 224.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-04	8.800E-02	ns	I310	0 0 0 0 0	

1433. $C_8H_8N_4O_4S_3$
CL 11366
RN: **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E-03	4.500E-01	ns	M032	0 0 0 0 1	

1434. $C_8H_8N_4O_4S_3$
Benzolamide
2-Benzenesulfonamide-1,3,4-thiadiazole-5-sulfonamide
5-Benzenesulfonamido-1,3,4-thiadiazole-2-sulfonamide
1,3,4-Thiadiazole-2-sulfonamide, 5-[(phenylsulfonyl)amino]-
1,3,4-Thiadiazole-2-sulfonamide, 5-benzenesulfonamido-
RN: 3368-13-6 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:** 585.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.844E-01	25	C415	1 0 0 1 0	

1435. $C_8H_8N_4O_6$
2,4,6-Trinitroethylaniline
2-4-6-Trinitromonoethylaniline
RN: 7449-27-6 **MP** (°C)**:**
MW: 256.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.904E-04	1.000E-01	19	D067	1 2 0 0 2	
1.210E-03	3.100E-01	50	D067	1 2 0 0 2	
5.699E-03	1.460E+00	100	D067	1 2 0 0 2	

1436. C_8H_8O
Acetophenone
Acetophenon
Methyl phenyl ketone
RN: 98-86-2 **MP** (°C)**:** 20.05
MW: 120.15 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.503E-02	5.411E+00	24	H106	1 0 2 2 2	
4.611E-02	5.540E+00	24	M303	1 0 1 1 2	
5.243E-02	6.300E+00	25	A003	1 2 1 2 2	
4.470E-02	5.371E+00	25	B019	1 0 1 2 0	
4.470E-02	5.371E+00	25	B092	2 1 1 1 1	
9.600E-02	1.153E+01	25	D407	1 0 2 2 2	
5.600E-03	6.729E-01	25	F063	1 1 0 0 1	
6.605E-02	7.937E+00	60	B092	2 1 1 1 1	

1437. C_8H_8O
Styrene oxide
1,2-Epoxyethylbenzene
RN: 96-09-3 **MP** (°C)**:** –36.8
MW: 120.15 **BP** (°C)**:** 194.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-02	2.792E+00	25	I313	0 0 0 0 0	

1438. C_8H_8O
2,2,3-Trimethyl-3-pentanol
2,2,3-Trimethylpentanol-3
RN: 7294-05-5 **MP** (°C)**:** –6
MW: 120.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.120E+00	4.950E+02	20	G007	1 2 0 1 2	
4.119E+00	4.949E+02	25	G007	1 2 0 1 2	
4.119E+00	4.949E+02	30	G007	1 2 0 1 2	

1439. C_8H_8O
4-Methylbenzaldehyde
p-Methylbenzaldehyde
RN: 104-87-0 **MP** (°C)**:**
MW: 120.15 **BP** (°C)**:** 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	2.271E+00	25	M017	1 2 0 1 2	

1440. $C_8H_8O_2$
2′-Hydroxyacetophenone
1-(2-Hydroxyphenyl)ethanone
2-Acetylphenol
RN: 118-93-4 **MP** (°C)**:** 6
MW: 136.15 **BP** (°C)**:** 213 at 717 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	6.808E+00	30	K441	0 0 0 0 0	
1.100E-01	1.498E+01	40	K441	0 0 0 0 0	
1.400E-01	1.906E+01	50	K441	0 0 0 0 0	

1441. $C_8H_8O_2$
4-Hydroxyacetophenone
4′-Hydroxy-acetophenon
RN: 99-93-4 **MP** (°C)**:** 110
MW: 136.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.271E-02	9.900E+00	22	F300	1 0 0 0 1	
7.000E-02	9.531E+00	30	K441	0 0 0 0 0	
1.400E-01	1.906E+01	40	K441	0 0 0 0 0	
1.800E-01	2.451E+01	50	K441	0 0 0 0 0	

1442. $C_8H_8O_2$
p-Anisaldehyde
Anisaldehyd
p-Methoxybenzaldehyde
RN: 123-11-5 **MP** (°C)**:** 0
MW: 136.15 **BP** (°C)**:** 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-02	2.000E+00	20	F300	1 0 0 0 0	
3.900E-02	5.310E+00	25	D407	1 0 2 2 2	
3.150E-02	4.289E+00	25	I019	1 0 1 2 2	

1443. $C_8H_8O_2$
m-Toluic acid
3-Methylbenzoic acid
m-Methylbenzoic acid
β-Methylbenzoic acid
RN: 99-04-7 **MP** (°C)**:** 112
MW: 136.15 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	9.803E-01	25	F001	1 0 1 0 2	
7.198E-03	9.800E-01	25	F300	1 0 0 0 2	
7.785E-03	1.060E+00	37	M360	1 2 1 1 2	

1444. $C_8H_8O_2$
p-Toluic acid
4-Methylbenzoic acid
Toluenecarboxylic acid
RN: 99-94-5 **MP** (°C)**:** 180
MW: 136.15 **BP** (°C)**:** 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	3.404E-01	25	F001	1 0 1 0 2	
2.938E-03	4.000E-01	25	F300	1 0 0 0 2	
2.277E-03	3.100E-01	37	M360	1 2 1 1 2	
2.780E-03	3.785E-01	ns	C014	0 0 0 1 2	

1445. $C_8H_8O_2$
o-Toluic acid
o-Tolylsaeure
o-Toluylic acid
2-Methylbenzoic acid
RN: 118-90-1 **MP** (°C)**:** 107
MW: 136.15 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-03	1.185E+00	25	F001	1 0 1 0 2	
8.780E-03	1.195E+00	25	R016	0 0 0 0 0	
1.014E-02	1.380E+00	37	M360	1 2 1 1 2	

1446. $C_8H_8O_2$
Phenylacetic acid
Phenylessigsaeure
RN: 103-82-2 **MP** (°C)**:** 76.5
MW: 136.15 **BP** (°C)**:** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-01	1.600E+01	20	F071	1 1 2 1 2	
1.219E-01	1.660E+01	20	H080	1 0 0 0 2	
1.219E-01	1.660E+01	20	M344	1 0 0 0 2	
1.300E-01	1.770E+01	25	F300	1 0 0 0 2	
1.267E-01	1.725E+01	25	H071	2 2 2 1 2	
1.310E-01	1.784E+01	25	K040	1 0 2 1 2	
1.300E-01	1.770E+01	25.00	M135	1 2 1 1 2	0.01N sodium phenylacetate
1.451E-01	1.975E+01	30	D033	2 2 1 2 2	
1.910E-01	2.600E+01	35.00	M135	1 2 1 1 2	
2.113E-01	2.877E+01	40	D033	2 2 1 2 2	
2.880E-01	3.921E+01	41.50	M135	1 2 1 1 2	
2.900E-01	3.948E+01	45.00	M135	1 2 1 1 2	
3.650E-01	4.970E+01	58.40	M135	1 2 1 1 2	

(*continued*)

1446. $C_8H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-01	5.923E+01	68.80	M135	1 2 1 1 2	
5.130E-01	6.985E+01	76.50	M135	1 2 1 1 2	
6.110E-01	8.319E+01	83.00	M135	1 2 1 1 2	
6.860E-01	9.340E+01	86.70	M135	1 2 1 1 2	
7.712E-01	1.050E+02	100	F300	1 0 0 0 2	
1.259E-01	1.714E+01	ns	R424	0 0 0 0 0	

1447. $C_8H_8O_2$

Methyl benzoate
Methyl *p*-hydroxybenzoate

RN: 93-58-3 **MP** (°C)**:** –12
MW: 136.15 **BP** (°C)**:** 198

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.337E-03	9.990E-01	15	G040	1 0 2 0 0	
3.085E-02	4.200E+00	22	N317	1 1 2 1 2	
2.926E-02	3.984E+00	25	G040	1 0 2 0 0	
1.447E-02	1.970E+00	25	L086	1 0 1 1 2	
1.497E-02	2.038E+00	25	M334	1 0 1 1 2	
1.777E-02	2.420E+00	30	L012	2 0 2 2 2	
1.796E-02	2.445E+00	30	L086	1 0 1 1 2	
3.654E-02	4.975E+00	35	G040	1 0 2 0 0	
2.221E-02	3.024E+00	35	L086	1 0 1 1 2	
2.723E-02	3.708E+00	40	L086	1 0 1 1 2	

1448. $C_8H_8O_2Hg$

Phenylmercuric acetate
Ceresan
PMAC
Acetate, phenylmercuric
PMA

RN: 62-38-4 **MP** (°C)**:** 149
MW: 336.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-02	2.470E+01	20	M061	1 0 0 0 2	
1.389E-02	4.678E+00	ns	B185	0 0 0 0 0	
1.396E-02	4.700E+00	ns	N013	0 0 0 0 2	
1.298E-02	4.370E+00	rt	M161	0 0 0 0 2	

1449. $C_8H_8O_3$
Methyl salicylate
Salicylsaeure-methyl ester
Methyl hydroxybenzoate
Betula oil
Panalgesic
Betula
RN: 119-36-8 **MP** (°C)**:** –8
MW: 152.15 **BP** (°C)**:** 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.206E-03	6.400E-01	21	B331	0 0 0 0 0	
4.000E-03	6.086E-01	25	D407	1 0 2 2 2	
1.312E-02	1.996E+00	25	R041	0 0 0 0 0	
4.601E-03	7.000E-01	30	F300	1 0 0 0 0	
6.244E-03	9.500E-01	30	L012	2 0 2 2 1	

1450. $C_8H_8O_3$
Vanillin
4-Hydroxy-3-methoxybenzaldehyde
3-Methoxy-4-hydroxybenzaldehyde
Methylprotocatechuic aldehyde
Vanillic aldehyde
Vanillaldehyde
RN: 121-33-5 **MP** (°C)**:** 82
MW: 152.15 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-02	6.754E+00	.2	D073	1 1 2 1 1	
1.972E-02	3.000E+00	4.40	M096	1 1 2 1 1	
3.418E-02	5.200E+00	15.60	M096	1 1 2 1 2	
8.114E-02	1.235E+01	20	D073	1 1 2 1 2	
6.572E-02	1.000E+01	20	F300	1 0 0 0 0	
5.915E-02	9.000E+00	23.90	M096	1 1 2 1 2	
4.800E-02	7.303E+00	25	D407	1 0 2 2 2	
7.240E-02	1.102E+01	25	I019	1 0 1 2 2	
9.713E-02	1.478E+01	30	D073	1 1 2 1 2	
8.500E-02	1.293E+01	30	L069	1 0 1 1 0	EFG
1.697E-01	2.582E+01	40	D073	1 1 2 1 2	
3.010E-01	4.580E+01	50	D073	1 1 2 1 2	
3.160E-01	4.807E+01	60	D073	1 1 2 1 2	
3.286E-01	5.000E+01	80	F300	1 0 0 0 0	

1451. $C_8H_8O_3$

Methylparaben
Me-paraben
Methyl *p*-hydroxybenzoic acid
Methyl 4-hydroxybenzoate
Methyl paraben

RN: 99-76-3 **MP** (°C)**:** 131
MW: 152.15 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.310E-03	1.264E+00	15	B355	0 0 0 0 0	
1.026E-02	1.561E+00	15	M352	1 1 1 1 2	
9.970E-03	1.517E+00	20	B355	0 0 0 0 0	
1.334E-02	2.030E+00	20	H056	1 0 2 1 2	
1.441E-02	2.193E+00	25	A059	1 0 1 1 2	
1.140E-02	1.735E+00	25	B355	0 0 0 0 0	
1.639E-02	2.494E+00	25	D081	1 2 2 1 2	
1.600E-02	2.434E+00	25	D339	0 0 0 0 0	
3.162E-02	4.811E+00	25	F322	2 0 1 1 0	EFG
1.364E-02	2.075E+00	25	L075	1 0 1 1 2	
1.393E-02	2.120E+00	25	L338	1 0 1 1 2	
1.460E-02	2.221E+00	25	M014	2 0 1 1 2	
1.585E-02	2.412E+00	25	M352	1 1 1 1 2	
1.643E-02	2.500E+00	25	O027	1 0 1 0 1	
1.485E-02	2.260E+00	25	P013	0 0 0 0 0	
1.446E-02	2.200E+00	25	P053	1 0 1 1 2	
1.600E-02	2.434E+00	27	B129	2 2 2 2 2	
1.500E-02	2.282E+00	27	G078	2 1 0 1 0	EFG
1.600E-02	2.434E+00	27	P019	1 2 1 1 0	EFG
1.450E-02	2.206E+00	27.0	G067	2 0 1 1 2	
1.828E-02	2.782E+00	30	A059	1 0 1 1 2	
1.564E-02	2.380E+00	30	M325	1 0 0 0 1	
2.275E-02	3.462E+00	35	A059	1 0 1 1 2	
2.550E-02	3.880E+00	37	B171	2 0 1 1 2	
2.268E-02	3.451E+00	39.3	G302	2 2 2 2 0	EFG
2.551E-02	3.882E+00	40	A059	1 0 1 1 2	
3.773E-02	5.740E+00	40	M352	1 1 1 1 2	
4.168E-02	6.341E+00	50	M352	1 1 1 1 2	

1452. $C_8H_8O_3$

D-Mandelic acid
(*R*)(–)Mandelic acid
(*S*)-α-Hydroxybenzeneacetic acid
L-Mandelic acid
(*S*)-(+)-Mandelic acid

RN: 17199-29-0 **MP** (°C)**:** 132
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.310E-01	8.080E+01	0	A043	1 2 1 1 2	
5.310E-01	8.080E+01	0	L035	1 2 2 1 2	

(*continued*)

1452. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-01	1.046E+02	10	A043	1 2 1 1 2	
6.874E-01	1.046E+02	10	L035	1 2 2 1 2	
7.766E-01	1.182E+02	15	A043	1 2 1 1 2	
7.766E-01	1.182E+02	15	L035	1 2 2 1 2	
9.158E-01	1.393E+02	20	A043	1 2 1 1 2	
9.158E-01	1.393E+02	20	L035	1 2 2 1 2	
5.371E-01	8.173E+01	24.5	L035	1 2 2 1 1	
5.371E-01	8.173E+01	24.50	A043	1 2 1 1 1	
1.183E+00	1.800E+02	25	A043	1 2 1 1 2	
6.503E-01	9.894E+01	25	C045	2 2 0 1 2	
6.705E-01	1.020E+02	25	C045	2 2 0 1 2	
1.183E+00	1.800E+02	25	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.5	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.50	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.5	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.50	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	L035	1 2 2 1 2	
3.434E+00	5.224E+02	37	A043	1 2 1 1 2	
1.132E+00	1.722E+02	37	A043	1 2 1 1 2	
3.434E+00	5.224E+02	37	L035	1 2 2 1 2	
1.132E+00	1.722E+02	37	L035	1 2 2 1 2	
4.075E+00	6.201E+02	40	A043	1 2 1 1 2	
4.075E+00	6.201E+02	40	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.5	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.50	A043	1 2 1 1 2	
4.325E+00	6.580E+02	42.5	L035	1 2 2 1 2	
4.325E+00	6.580E+02	42.50	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45.50	A043	1 2 1 1 2	
2.351E+00	3.577E+02	46.5	L035	1 2 2 1 2	
2.351E+00	3.577E+02	46.50	A043	1 2 1 1 2	
4.816E+00	7.328E+02	47	L035	1 2 2 1 2	
4.816E+00	7.328E+02	47.50	A043	1 2 1 1 2	
2.795E+00	4.253E+02	48.5	L035	1 2 2 1 2	
2.795E+00	4.253E+02	48.50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.5	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.50	A043	1 2 1 1 2	
3.484E+00	5.301E+02	52.5	L035	1 2 2 1 2	
3.484E+00	5.301E+02	52.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	L035	1 2 2 1 2	
3.996E+00	6.080E+02	57	A043	1 2 1 1 2	

(*continued*)

1452. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.996E+00	6.080E+02	57	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.5	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.50	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	L035	1 2 2 1 2	

1453. $C_8H_8O_3$

m-Cresotic acid
2-Hydroxy-*p*-tolylsaeure-(1)
m-Kresotinsaeure

RN: 50-85-1 **MP** (°C)**:** 177
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.638E-02	1.010E+01	100	F300	1 0 0 0 2	

1454. $C_8H_8O_3$

o-Anisic acid
2-Methoxybenzoic acid
Salicylic acid methyl ether
Salicylsaeure-methylaether
o-Methoxybenzoic acid

RN: 579-75-9 **MP** (°C)**:** 101
MW: 152.15 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-02	1.567E+00	4.99	A405	2 0 1 1 2	
1.220E-02	1.856E+00	9.99	A405	2 0 1 1 2	
1.420E-02	2.161E+00	14.99	A405	2 0 1 1 2	
1.710E-02	2.602E+00	19.99	A405	2 0 1 1 2	
2.070E-02	3.150E+00	23.99	A405	2 0 1 1 2	
2.760E-02	4.200E+00	25	H007	0 0 0 0 0	
2.440E-02	3.712E+00	26.99	A405	2 0 1 1 2	
3.286E-02	5.000E+00	30	F300	1 0 0 0 0	
2.760E-02	4.199E+00	30.99	A405	2 0 1 1 2	
3.120E-02	4.747E+00	34.99	A405	2 0 1 1 2	
3.503E-02	5.330E+00	37	M360	1 2 1 1 2	
3.750E-02	5.706E+00	38.99	A405	2 0 1 1 2	
4.390E-02	6.679E+00	41.99	A405	2 0 1 1 2	
4.800E-02	7.303E+00	44.99	A405	2 0 1 1 2	
5.930E-02	9.023E+00	47.99	A405	2 0 1 1 2	
6.930E-02	1.054E+01	52.99	A405	2 0 1 1 2	
8.370E-02	1.274E+01	53.99	A405	2 0 1 1 2	
9.500E-02	1.445E+01	56.99	A405	2 0 1 1 2	
1.261E-01	1.919E+01	60.99	A405	2 0 1 1 2	
1.683E-01	2.561E+01	64.99	A405	2 0 1 1 2	

(*continued*)

1454. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.326E-01	3.539E+01	68.99	A405	2 0 1 1 2	
2.630E-01	4.002E+01	69.99	A405	2 0 1 1 2	
3.467E-01	5.275E+01	72.99	A405	2 0 1 1 2	

1455. $C_8H_8O_3$
Mandelic acid
Amygdalic acid
α-Hydroxyphenylacetic acid
Uromaline
α-Hydroxy-benzeneacetic acid
RN: 90-64-2 **MP** (°C)**:** 119.0
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.191E+00	1.812E+02	25	K040	1 0 2 1 2	*sic*
8.795E-03	1.338E+00	25	R049	0 0 0 0 0	
9.120E-01	1.388E+02	ns	R427	0 0 0 0 0	

1456. $C_8H_8O_3$
3-Hydroxy-*p*-toluic acid
3-Hydroxy-*p*-tolylsaeure-(1)
RN: 586-30-1 **MP** (°C)**:**
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.859E-01	4.350E+01	100	F300	1 0 0 0 2	

1457. $C_8H_8O_3$
3-Methoxybenzoic acid
3-Methoxy-benzoesaeure
m-Anisic acid
m-Methoxybenzoic acid
RN: 586-38-9 **MP** (°C)**:** 110
MW: 152.15 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.282E-02	1.950E+00	37	M360	1 2 1 1 2	
1.183E-03	1.800E-01	ns	B361	0 0 0 0 0	

1458. $C_8H_8O_3$
DL-Mandelic acid
DL-Mandelsaeure
RN: 611-72-3 **MP** (°C)**:** 122
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.050E-01	1.377E+02	20	F300	1 0 0 0 2	
1.134E+00	1.725E+02	24	F300	1 0 0 0 2	

1459. $C_8H_8O_3$
4-Hydroxy-*m*-toluic acid
4-Hydroxy-*m*-tolylsaeure-(1)
o-Cresotic acid
2-Hydroxy-*m*-toluic acid
2-Hydroxy-*m*-tolylsaeure-(1)
RN: 83-40-9 **MP** (°C)**:** 165.5
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-02	1.160E+01	100	F300	1 0 0 0 2	
3.411E-01	5.190E+01	100	F300	1 0 0 0 2	

1460. $C_8H_8O_3$
Phenoxyacetic acid
Glycolic acid phenyl ether
O-Phenylglycolic acid
RN: 122-59-8 **MP** (°C)**:** 98
MW: 152.15 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.887E-02	1.200E+01	10	F071	1 1 2 1 2	
8.084E-03	1.230E+00	10	F300	1 0 0 0 2	
7.887E-02	1.200E+01	10	H080	1 0 0 0 2	
7.887E-02	1.200E+01	10	M344	1 0 0 0 2	
1.100E-04	1.674E-02	25	L030	1 0 2 1 2	

1461. $C_8H_8O_3$
p-Methoxybenzoic acid
4-Methoxybenzoic acid
p-Anisic acid
Anissaeure
RN: 100-09-4 **MP** (°C)**:** 184
MW: 152.15 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.111E-01	2.99	A405	2 0 1 1 2	
9.400E-04	1.430E-01	4.99	A405	2 0 1 1 2	
1.070E-03	1.628E-01	10.99	A405	2 0 1 1 2	
1.270E-03	1.932E-01	14.99	A405	2 0 1 1 2	
1.775E-02	2.700E+00	19	F300	1 0 0 0 1	
1.330E-03	2.024E-01	19.99	A405	2 0 1 1 2	
1.680E-03	2.556E-01	24.99	A405	2 0 1 1 2	
2.020E-03	3.073E-01	28.99	A405	2 0 1 1 2	
2.300E-03	3.499E-01	33.99	A405	2 0 1 1 2	
3.483E-03	5.300E-01	37	B171	2 0 1 1 2	
1.380E-03	2.100E-01	37	M360	1 2 1 1 2	
3.110E-03	4.732E-01	39.99	A405	2 0 1 1 2	
3.870E-03	5.888E-01	43.99	A405	2 0 1 1 2	
5.130E-03	7.805E-01	50.99	A405	2 0 1 1 2	
6.110E-03	9.296E-01	55.99	A405	2 0 1 1 2	
8.170E-03	1.243E+00	59.99	A405	2 0 1 1 2	
9.000E-03	1.369E+00	64.99	A405	2 0 1 1 2	
1.080E-02	1.643E+00	65.99	A405	2 0 1 1 2	
1.100E-02	1.674E+00	66.99	A405	2 0 1 1 2	
1.460E-02	2.221E+00	71.99	A405	2 0 1 1 2	
1.778E-02	2.706E+00	ns	R427	0 0 0 0 0	

1462. $C_8H_8O_3$
p-Cresotic acid
6-Hydroxy-*m*-toluic acid
6-Hydroxy-*m*-tolylsaeure-(1)
RN: 89-56-5 **MP** (°C)**:** 151
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	2.190E+01	100	F300	1 0 0 0 2	

1463. $C_8H_8O_4$
Vanillic acid
Vanillinsaeure
RN: 121-34-6 **MP** (°C)**:** 214
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.921E-03	1.500E+00	14	F300	1 0 0 0 1	
1.546E-01	2.600E+01	100	F300	1 0 0 0 2	

1464. $C_8H_8O_4$
Homogentisic acid
2,5-Dihydroxyphenylacetic acid
2,5-Dihydroxy-benzeneacetic acid
RN: 451-13-8 **MP** (°C)**:** 151
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.732E+00	4.595E+02	25	D041	1 0 0 0 1	

1465. $C_8H_8O_5$
Methyl gallate
Gallussaeuremethyl ester
Methyl-3,4,5-trihydroxybenzoate
RN: 99-24-1 **MP** (°C)**:** 201.5
MW: 184.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.323E-02	9.803E+00	19.99	L430	0 0 0 0 0	
5.696E-02	1.049E+01	24.99	L430	0 0 0 0 0	
6.757E-02	1.244E+01	29.99	L430	0 0 0 0 0	
9.549E-02	1.759E+01	34.99	L430	0 0 0 0 0	
1.340E-01	2.468E+01	39.99	L430	0 0 0 0 0	
1.704E-01	3.138E+01	44.99	L430	0 0 0 0 0	
2.542E-01	4.680E+01	49.99	L430	0 0 0 0 0	
4.328E-01	7.970E+01	54.99	L430	0 0 0 0 0	
5.879E-01	1.083E+02	59.99	L430	0 0 0 0 0	
7.775E-01	1.432E+02	64.99	L430	0 0 0 0 0	
1.054E+00	1.941E+02	69.99	L430	0 0 0 0 0	
1.624E-02	2.991E+00	–.0	L430	0 0 0 0 0	
5.756E-02	1.060E+01	ns	F300	0 0 0 0 2	

1466. $C_8H_9ClNO_5PS$

Chlorthion
O,O-Dimethyl *O*-4-nitro-3-chlorophenyl thiophosphate
RN: 500-28-7 **MP** (°C)**:** 21
MW: 297.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.344E-04	4.000E-02	20	M061	1 0 0 0 1	

1467. $C_8H_9ClNO_5PS$

Dicapthon
O-(2-Chloro-4-nitrophenyl) *O,O*-dimethyl phosphorothioate
Dicaptan
Isochlorthion
RN: 2463-84-5 **MP** (°C)**:**
MW: 297.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B300	2 1 1 1 2	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
2.100E-05	6.250E-03	20	C053	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
2.100E-05	6.250E-03	ns	F071	0 1 2 1 2	
1.176E-04	3.500E-02	ns	M061	0 0 0 0 1	
2.620E-05	7.800E-03	rt	F040	1 2 2 2 1	

1468. C_8H_9ClO

2,5-Dimethyl-4-chloro-phenol
4-Chloro-2,5-xylenol
4-Chloro-2,5-dimethylphenol
RN: 1124-06-7 **MP** (°C)**:** 114–116
MW: 156.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	8.927E+00	25	B316	0 0 0 0 0	

1469. C_8H_9ClO

2,6-Dimethyl-4-chloro-phenol
4-Chloro-2,6-xylenol
RN: 1123-63-3 **MP** (°C)**:**
MW: 156.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-03	5.168E-01	25	B316	0 0 0 0 0	

1470. C_8H_9ClO
Chloroxylenol
3,5-Dimethyl-4-chloro-phenol-
RN: 88-04-0 **MP** (°C)**:** 115.5
MW: 156.61 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	2.500E-01	20	M018	1 2 2 1 0	EFG
1.979E-03	3.099E-01	20	M093	1 0 0 1 1	
2.200E-02	3.445E+00	25	B316	0 0 0 0 0	*sic*
1.915E-03	2.999E-01	25	R041	0 0 0 0 0	
1.585E-03	2.482E-01	ns	R427	0 0 0 0 0	

1471. $C_8H_9FN_2O_3$
2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxobutyl)-
RN: 94452-21-8 **MP** (°C)**:**
MW: 200.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-02	1.061E+01	22	B416	2 2 1 2 1	

1472. $C_8H_9FN_2O_3$
Ftorafur
THFFU
1-(2-Tetrahydrofuryl)-5-fluorouracil
RN: 37076-68-9 **MP** (°C)**:** 167
MW: 200.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	2.802E+01	37	N017	0 0 0 0 0	

1473. $C_8H_9FN_2O_4$
1-Propionyloxymethyl-5-fluorouracil
1-Propionyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
RN: 66542-36-7 **MP** (°C)**:** 100–102
MW: 216.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-01	3.360E+01	22	B321	0 0 0 0 0	pH 4.0

1474. $C_8H_9FN_2O_4$
1-Isopropyloxyarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 1-methylethyl ester
RN: 109232-73-7 **MP** (°C)**:** 180
MW: 216.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E-02	4.700E+00	22	B332	1 1 0 0 1	pH 4.0

1475. C_8H_9N
Indoline
2,3-Dihydro-1H-indole
2,3-Dihydroindole
RN: 496-15-1 **MP** (°C)**:** <25
MW: 119.17 **BP** (°C)**:** 220.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.934E-02	3.497E+00	20.3	L339	2 0 2 2 2	
9.063E-02	1.080E+01	25	P051	2 1 1 2 2	
9.063E-02	1.080E+01	25.00	P007	2 1 2 2 1	
3.651E-02	4.350E+00	40.0	L339	2 0 2 2 2	
4.586E-02	5.465E+00	59.4	L339	2 0 2 2 2	
5.738E-02	6.838E+00	79.0	L339	2 0 2 2 2	
8.142E-02	9.703E+00	100.0	L339	2 0 2 2 2	

1476. C_8H_9NO
p-Aminoacetophenone
4′-Aminoacetophenone
RN: 99-92-3 **MP** (°C)**:** 106
MW: 135.17 **BP** (°C)**:** 294

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.480E-02	3.352E+00	37.5	G002	1 1 1 1 2	

1477. C_8H_9NO
Acetanilide
Acetanilid
RN: 103-84-4 **MP** (°C)**:** 114
MW: 135.17 **BP** (°C)**:** 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.652E-02	3.585E+00	0	L029	2 2 2 2 2	
3.534E-02	4.777E+00	10	M043	1 0 0 0 1	
3.251E-02	4.395E+00	10.1	L029	2 2 2 2 2	
2.970E-02	4.014E+00	14	O016	1 0 0 0 2	
3.688E-02	4.985E+00	15	L038	1 0 1 0 2	

(*continued*)

1477. C_8H_9NO (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-02	5.015E+00	20	B101	0 0 0 0 0	
3.666E-02	4.955E+00	20	K078	1 0 2 1 2	
4.129E-02	5.581E+00	20	L029	2 2 2 2 2	
3.827E-02	5.173E+00	20	M043	1 0 0 0 1	
3.330E-02	4.501E+00	20	O019	1 0 0 1 2	
3.884E-02	5.250E+00	20	W026	1 0 1 1 1	average of 2
4.142E-02	5.598E+00	25	B101	0 0 0 0 0	
4.450E-02	6.015E+00	25	B434	0 0 0 0 0	
4.786E-02	6.468E+00	25	B434	0 0 0 0 0	
4.160E-02	5.623E+00	25	D044	0 0 0 0 0	
4.143E-02	5.600E+00	25	F300	1 0 0 0 1	
4.697E-02	6.349E+00	25	L029	2 2 2 2 2	
4.486E-02	6.063E+00	25	M094	1 0 0 1 1	
3.699E-02	5.000E+00	25	P016	1 0 0 1 0	
4.887E-02	6.606E+00	30	B101	0 0 0 0 0	
5.262E-02	7.113E+00	30	B434	0 0 0 0 0	
5.240E-02	7.083E+00	30	B434	0 0 0 0 0	
5.351E-02	7.232E+00	30	L029	2 2 2 2 2	
4.632E-02	6.261E+00	30	M043	1 0 0 0 1	
5.253E-02	7.100E+00	30	W026	1 0 1 1 1	average of 2
5.792E-02	7.828E+00	32.6	L038	1 0 1 0 2	
5.930E-02	8.015E+00	35	B101	0 0 0 0 0	
5.799E-02	7.838E+00	35	B434	0 0 0 0 0	
5.760E-02	7.786E+00	35	B434	0 0 0 0 0	
6.787E-02	9.174E+00	40	B434	0 0 0 0 0	
6.730E-02	9.097E+00	40	B434	0 0 0 0 0	
7.134E-02	9.643E+00	40	L029	2 2 2 2 2	
6.381E-02	8.625E+00	40	M043	1 0 0 0 1	
9.682E-02	1.309E+01	50	L029	2 2 2 2 2	
1.349E-01	1.823E+01	60	L029	2 2 2 2 2	
1.522E-01	2.057E+01	60	M043	1 0 0 0 1	
1.928E-01	2.606E+01	70	L029	2 2 2 2 2	
3.321E-01	4.489E+01	80	M043	1 0 0 0 1	
4.047E-02	5.470E+00	rt	D021	0 0 1 1 1	

1478. C_8H_9NO

m-Aminoacetophenone
3′-Aminoacetophenone

RN: 99-03-6 **MP** (°C)**:** 97
MW: 135.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.220E-02	7.056E+00	37.5	G002	1 1 1 1 2	pH 6.8

1479. $C_8H_9NO_2$
Acetaminophen
4-Acetamidophenol
4-Amino-phenol-*N*-acetat
p-Acetaminophen
p-Hydroxyacetanilide
RN: 103-90-2 **MP** (°C)**:** 167
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.307E-02	1.105E+01	15	M352	1 1 1 1 2	
5.462E-01	8.257E+01	16.9	Y412	0 0 0 0 0	
6.014E-01	9.091E+01	21.5	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	25	B010	1 1 1 1 0	
1.016E-01	1.536E+01	25	B434	0 0 0 0 0	
9.500E-02	1.436E+01	25	C032	2 2 1 2 0	EFG
7.710E-02	1.165E+01	25	D044	0 0 0 0 0	
9.133E-02	1.381E+01	25	D078	1 2 1 1 2	
5.185E-02	7.838E+00	25	F415	0 0 0 0 0	Average
1.000E-01	1.512E+01	25	K041	1 0 0 0 0	
9.851E-02	1.489E+01	25	M352	1 1 1 1 2	
9.923E-02	1.500E+01	25	P016	1 0 0 1 1	
7.277E-02	1.100E+01	25	P312	0 0 0 0 0	
9.326E-02	1.410E+01	25	W019	1 0 1 1 2	
3.538E-01	5.348E+01	25	Y410	0 0 0 0 0	
9.140E-02	1.382E+01	25	Z408	0 0 0 0 0	
6.556E-01	9.910E+01	26.3	Y412	0 0 0 0 0	
1.241E-01	1.876E+01	30	B434	0 0 0 0 0	
1.240E-01	1.874E+01	30	B434	0 0 0 0 0	
1.120E-01	1.693E+01	30	L069	1 0 1 1 0	EFG
7.088E-01	1.071E+02	31.5	Y412	0 0 0 0 0	
1.684E-01	2.545E+01	35	B434	0 0 0 0 0	
1.684E-01	2.546E+01	35	B434	0 0 0 0 0	
7.610E-01	1.150E+02	35.3	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	37	F076	2 0 2 2 0	
1.442E-01	2.180E+01	37	K086	1 0 0 0 2	
8.124E-01	1.228E+02	37	Y412	0 0 0 0 0	
1.349E-01	2.039E+01	39.3	G302	2 0 2 2 0	EFG
2.234E-01	3.377E+01	40	B434	0 0 0 0 0	
2.238E-01	3.384E+01	40	B434	0 0 0 0 0	
1.440E-01	2.177E+01	40	M352	1 1 1 1 2	
1.800E-01	2.720E+01	50	M352	1 1 1 1 2	
1.019E-01	1.540E+01	c	B434	0 0 0 0 0	
6.615E-04	1.000E-01	ns	K444	0 0 0 0 0	
8.004E-02	1.210E+01	rt	R431	0 0 0 0 0	Average

1480. $C_8H_9NO_2$
Benzyl carbamate
O-Benzyl carbamate
Benzyloxycarbonyl amine
RN: 621-84-1 **MP** (°C)**:** 87
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-01	6.802E+01	37	H006	1 2 2 1 1	
4.467E-01	6.752E+01	ns	R427	0 0 0 0 0	

1481. $C_8H_9NO_2$
DL-2-Phenylglycine
2-Amino-phenyl-essigsaeure
2-Aminophenylacetic acid
RN: 2835-06-5 **MP** (°C)**:** 255
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.608E-01	1.150E+02	100	F300	1 0 0 0 2	

1482. $C_8H_9NO_2$
N-Methylanthranilic acid
N-Methyl-anthranilsaeure
RN: 119-68-6 **MP** (°C)**:** 171
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-03	2.000E-01	20	F300	1 0 0 0 2	
2.646E-03	4.000E-01	100	F300	1 0 0 0 2	

1483. $C_8H_9NO_2$
D-Phenylglycine
D-2-Phenylglycine
D-(–)-α-Aminophenylacetic acid
Benzeneacetic acid, α-amino-
RN: 875-74-1 **MP** (°C)**:** 302 C
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-02	4.586E+00	25	R419	0 0 0 0 0	

1484. $C_8H_9NO_2$

Methyl-*p*-aminobenzoate
Methyl *p*-aminobenzoate
4-Aminobenzoic acid methyl ester
RN: 619-45-4 **MP** (°C)**:**
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.884E-03	8.894E-01	15	M352	1 1 1 1 2	
9.542E-03	1.442E+00	25	M352	1 1 1 1 2	
1.070E-02	1.618E+00	25	P303	0 0 0 0 0	
1.397E-02	2.112E+00	33	P303	0 0 0 0 0	
2.530E-02	3.825E+00	37	F006	1 1 2 2 2	
1.646E-02	2.488E+00	40	M352	1 1 1 1 2	
1.839E-02	2.780E+00	40	P303	0 0 0 0 0	
7.940E-03	1.200E+00	ns	M066	0 0 0 0 2	
7.940E-03	1.200E+00	rt	B016	0 0 1 1 2	pH 7.4

1485. $C_8H_9NO_2S_2$

2-(2-Thienyl)-L-thiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-(2-thienyl)-
RN: 32451-19-7 **MP** (°C)**:**
MW: 215.29 **BP** (°C)**:** 454.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.055E+00	21	B414	1 0 0 1 1	fast decomposition

1486. $C_8H_9NO_3$

D-(*p*-hydroxy)phenylglycine
RN: **MP** (°C)**:**
MW: 167.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-01	1.937E+01	25	R419	0 0 0 0 0	

1487. $C_8H_9NO_3S$

p-Acetylbenzenesulfonamide
4-Acetylbenzenesulfonamide
RN: 1565-17-9 **MP** (°C)**:**
MW: 199.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.582E-01	15	K024	1 2 1 1 2	

1488. $C_8H_9NO_4$
Biliverdic acid
Biliverdinsaeure
RN: 487-65-0 **MP** (°C)**:**
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-01	3.900E+01	20	F300	1 0 0 0 1	

1489. $C_8H_9N_3O_3$
Orotic acid allylamide
4-Pyrimidinecarboxamide, 1,2,3,6-tetrahydro-2,6-dioxo-*N*-2-propenyl-
RN: 292870-71-4 **MP** (°C)**:** 259–262
MW: 195.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-01	3.474E+01	−4	N018	0 0 0 0 0	
3.000E-01	5.855E+01	16	N018	0 0 0 0 0	
3.710E-01	7.241E+01	25	N018	0 0 0 0 0	

1490. $C_8H_9N_5$
7-Dimethylaminopteridine
7-Pteridinamine, *N,N*-dimethyl-
RN: 204443-26-5 **MP** (°C)**:**
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.154E-01	1.429E+02	20	A083	1 2 0 0 0	
1.903E+00	3.333E+02	100	A083	1 2 0 0 0	

1491. $C_8H_9N_5$
2-Dimethylaminopteridine
2-Pteridinamine, *N,N*-dimethyl-
RN: 41047-52-3 **MP** (°C)**:**
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.631E+00	2.857E+02	22.5	A085	1 2 0 0 0	

1492. $C_8H_9N_5$
4-Dimethylaminopteridine
4-Pteridinamine, *N,N*-dimethyl-
RN: 14131-04-5 **MP** (°C)**:** 165
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.357E-02	1.639E+01	20	A019	2 2 1 1 0	
1.392E-01	2.439E+01	100	A019	1 2 1 1 0	

1493. $C_8H_9O_3PS$
2-Methoxy-4H-benzo-1,3,2-dioxaphosphorin-2-thione
Dioxabenzofos
Salithion
Fenfosphorin
Dioxabenzophos
RN: 3811-49-2 **MP** (°C)**:** 55.5
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-04	5.800E-02	30	M161	1 0 0 0 1	

1494. C_8H_{10}
Ethylbenzene
Phenylethane
Ethylenzene
Ethylbenzol
EB
RN: 100-41-4 **MP** (°C)**:** –95
MW: 106.17 **BP** (°C)**:** 136.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.856E-03	1.970E-01	0	P003	2 2 2 2 2	
1.846E-03	1.960E-01	4.50	B086	2 1 2 2 2	
1.808E-03	1.920E-01	6.30	B086	2 1 2 2 2	
1.677E-03	1.781E-01	7.09	F418	0 0 0 0 0	
1.752E-03	1.860E-01	7.10	B086	2 1 2 2 2	
1.761E-03	1.870E-01	9	B086	2 1 2 2 2	
1.910E-03	2.028E-01	10	B149	2 1 1 2 2	
1.850E-03	1.964E-01	10	O312	2 2 0 2 2	
1.705E-03	1.810E-01	11.80	B086	2 1 2 2 2	
1.723E-03	1.830E-01	12.10	B086	2 1 2 2 2	
1.812E-03	1.924E-01	14	O312	2 2 0 2 2	
1.300E-03	1.380E-01	15	F001	1 0 1 2 1	
1.300E-03	1.380E-01	15	S006	1 0 0 0 1	
1.658E-03	1.760E-01	15	S203	1 1 2 1 2	
1.695E-03	1.800E-01	15.10	B086	2 1 2 2 2	

(*continued*)

1494. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.639E-03	1.740E-01	16.93	F418	0 0 0 0 0	
1.776E-03	1.886E-01	17	O312	2 2 0 2 2	
1.733E-03	1.840E-01	17.90	B086	2 1 2 2 2	
2.901E-03	3.080E-01	18	F185	1 0 0 0 2	
2.788E-03	2.960E-01	18	F185	1 0 0 0 2	
1.725E-03	1.831E-01	18	O312	2 2 0 2 2	
3.080E-03	3.270E-01	19	F185	1 0 0 0 2	
1.676E-03	1.779E-01	19	O312	2 2 0 2 2	
2.000E-03	2.123E-01	20	B149	2 1 1 2 2	
1.695E-03	1.800E-01	20	B356	0 0 0 0 0	
1.770E-03	1.879E-01	20	O312	2 2 0 2 2	
1.695E-03	1.800E-01	20.10	B086	2 1 2 2 1	
1.724E-03	1.830E-01	21	O312	2 2 0 2 2	
3.297E-03	3.500E-01	22	F185	1 0 0 0 2	
1.713E-03	1.819E-01	22	O312	2 2 0 2 2	
3.391E-03	3.600E-01	23	F185	1 0 0 0 2	
1.751E-03	1.859E-01	23.5	O312	2 2 0 2 2	
3.655E-03	3.880E-01	24	F185	1 0 0 0 2	
1.582E-03	1.680E-01	25	A002	1 2 1 1 2	
1.883E-03	2.000E-01	25	A094	1 0 0 0 0	
1.959E-03	2.080E-01	25	B003	2 2 2 2 2	
1.432E-03	1.520E-01	25	B060	2 0 1 1 1	
2.000E-03	2.123E-01	25	B153	2 1 1 1 2	
1.640E-03	1.741E-01	25	K001	1 0 2 1 2	
1.319E-03	1.400E-01	25	K072	1 0 1 1 1	
1.760E-03	1.869E-01	25	M342	1 0 1 1 2	
1.811E-03	1.923E-01	25	O312	2 2 0 2 2	
1.667E-03	1.770E-01	25	P003	2 2 2 2 2	
1.234E-03	1.310E-01	25	P051	2 1 1 2 2	
1.705E-03	1.810E-01	25	S203	1 1 2 1 2	
1.518E-03	1.612E-01	25	S358	2 1 2 2 2	
1.370E-03	1.455E-01	25	S359	2 1 2 2 2	
1.760E-03	1.869E-01	25	W300	2 2 2 2 2	
1.959E-03	2.080E-01	25.0	G035	1 0 0 0 2	
1.753E-03	1.861E-01	25.8	O312	2 2 0 2 2	
1.705E-03	1.810E-01	26.74	F418	0 0 0 0 0	
4.653E-03	4.940E-01	27	F185	1 0 0 0 2	
1.677E-03	1.780E-01	28	B348	2 1 2 2 2	
1.747E-03	1.855E-01	28	O312	2 2 0 2 2	
5.604E-03	5.950E-01	29	F185	1 0 0 0 2	
1.600E-03	1.698E-01	29.99	C350	0 0 0 0 0	
1.391E-03	1.477E-01	30	M311	1 1 2 2 2	
1.777E-03	1.887E-01	30	O312	2 2 0 2 2	
6.103E-03	6.480E-01	31	F185	1 0 0 0 2	
6.395E-03	6.790E-01	32	F185	1 0 0 0 2	
7.017E-03	7.450E-01	34	F185	1 0 0 0 2	
7.319E-03	7.770E-01	35	F185	1 0 0 0 2	
1.818E-03	1.930E-01	35	O312	2 2 0 2 2	
1.827E-03	1.940E-01	35	S203	1 1 2 1 2	

(*continued*)

1494. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.865E-03	8.350E-01	36	F185	1 0 0 0 2	
1.805E-03	1.917E-01	36.55	F418	0 0 0 0 0	
8.637E-03	9.170E-01	38	F185	1 0 0 0 2	
1.622E-03	1.722E-01	39.99	C350	0 0 0 0 0	
1.928E-03	2.047E-01	40	O312	2 2 0 2 2	
9.466E-03	1.005E+00	41	F185	1 0 0 0 2	
1.991E-03	2.114E-01	45	O312	2 2 0 2 2	
2.025E-03	2.150E-01	45	S203	1 1 2 1 2	
1.994E-03	2.117E-01	46.49	F418	0 0 0 0 0	
1.154E-02	1.225E+00	47	F185	1 0 0 0 2	
1.224E-02	1.300E+00	49	F185	1 0 0 0 2	
1.861E-03	1.976E-01	49.99	C350	0 0 0 0 0	
2.216E-03	2.353E-01	56.73	F418	0 0 0 0 0	
2.261E-03	2.400E-01	59.99	C350	0 0 0 0 0	
2.560E-03	2.718E-01	66.64	F418	0 0 0 0 0	
2.738E-03	2.907E-01	69.99	C350	0 0 0 0 0	
3.327E-03	3.532E-01	79.99	C350	0 0 0 0 0	
3.860E-03	4.098E-01	89.99	C350	0 0 0 0 0	
4.742E-03	5.035E-01	99.99	C350	0 0 0 0 0	
4.829E-03	5.127E-01	115.0	G035	1 0 0 0 2	
1.120E-02	1.189E+00	140.5	G035	1 0 0 0 2	
3.332E-02	3.537E+00	170.5	G035	1 0 0 0 2	
6.185E-02	6.567E+00	210.0	G035	1 0 0 0 2	
1.052E-01	1.116E+01	233.5	G035	1 0 0 0 2	
1.432E-03	1.520E-01	ns	H123	0 0 0 0 0	
6.300E-02	6.689E+00	ns	H307	0 0 0 0 0	
1.432E-03	1.520E-01	ns	M344	0 0 0 0 2	

1495. C_8H_{10}

m-Xylene
1,3-Xylene

RN: 108-38-3 **MP** (°C)**:** –47.4
MW: 106.17 **BP** (°C)**:** 139.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.846E-03	1.960E-01	0	P003	2 2 2 2 2	
1.463E-03	1.554E-01	20	M337	2 1 2 2 2	
1.629E-03	1.730E-01	25	A001	1 2 2 2 2	
1.846E-03	1.960E-01	25	B003	2 2 2 2 2	
1.262E-03	1.340E-01	25	K119	1 0 0 0 2	
1.510E-03	1.603E-01	25	M342	1 0 1 1 2	
1.526E-03	1.620E-01	25	P003	2 2 2 2 2	
1.262E-03	1.340E-01	25	P051	2 1 1 2 2	
1.375E-03	1.460E-01	25	S005	2 2 2 2 2	
1.375E-03	1.460E-01	25	S191	1 2 2 2 2	
1.375E-03	1.460E-01	25	S358	2 1 2 2 2	
1.330E-03	1.412E-01	25	S359	2 1 2 2 2	

(*continued*)

1495. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-03	1.603E-01	25	W300	2 2 2 2 2	
1.262E-03	1.340E-01	25.00	P007	2 1 2 2 2	
1.940E-03	2.059E-01	25.04	V013	2 2 2 2 2	
3.277E-03	3.479E-01	67.7	P005	1 1 2 1 2	
6.257E-03	6.643E-01	107.3	P005	1 1 2 1 2	
9.707E-03	1.031E+00	124.2	P005	1 1 2 1 2	
2.363E-02	2.509E+00	164.2	P005	1 1 2 1 2	
4.327E-02	4.594E+00	186.4	P005	1 1 2 1 2	
4.293E-02	4.557E+00	189.9	P005	1 1 2 1 2	
2.675E-01	2.840E+01	266.6	P005	1 1 2 1 2	
2.698E-01	2.865E+01	270.6	P005	1 1 2 1 2	

1496. C_8H_{10}

o-Xylene
1,2-Dimethylbenzene
1,2-Xylene

RN: 95-47-6 **MP** (°C)**:** –25
MW: 106.17 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.337E-03	1.420E-01	0	P003	2 2 2 2 2	
2.000E-03	2.123E-01	10	B149	2 1 1 2 2	
2.260E-03	2.399E-01	20	B149	2 1 1 2 2	
1.605E-03	1.704E-01	20	M337	2 1 2 2 2	
1.921E-03	2.040E-01	25	A001	1 2 2 2 2	
1.648E-03	1.750E-01	25	B060	2 0 1 1 1	
1.573E-03	1.670E-01	25	K119	1 0 0 0 2	
1.648E-03	1.750E-01	25	M001	2 1 2 2 2	
1.648E-03	1.750E-01	25	M002	2 1 2 2 2	
1.648E-03	1.750E-01	25	M040	1 0 0 1 2	
1.648E-03	1.750E-01	25	M130	1 0 0 0 2	
2.080E-03	2.208E-01	25	M342	1 0 1 1 2	
2.006E-03	2.130E-01	25	P003	2 2 2 2 2	
1.573E-03	1.670E-01	25	P051	2 1 1 2 2	
1.606E-03	1.705E-01	25	S005	2 2 2 2 2	
1.606E-03	1.705E-01	25	S191	1 2 2 2 2	
1.606E-03	1.705E-01	25	S358	2 1 2 2 2	
1.680E-03	1.784E-01	25	S359	2 1 2 2 2	
2.080E-03	2.208E-01	25	W300	2 2 2 2 2	
1.573E-03	1.670E-01	25.00	P007	2 1 2 2 2	
1.272E-03	1.350E-01	ns	B150	0 0 2 2 2	
1.648E-03	1.750E-01	ns	M344	0 0 0 0 2	

1497. C_8H_{10}
p-Xylene
1,4-Dimethylbenzene
1,4-Xylene
RN: 106-42-3 **MP** (°C)**:** 13
MW: 106.17 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.545E-03	1.640E-01	0	P003	2 2 2 2 2	
1.780E-03	1.890E-01	10	B149	2 1 1 2 2	
1.800E-03	1.911E-01	20	B149	2 1 1 2 2	
1.552E-03	1.648E-01	20	M337	2 1 2 2 2	
1.884E-03	2.000E-01	25	A001	1 2 2 2 2	
1.865E-03	1.980E-01	25	B003	2 2 2 2 2	
1.224E-03	1.300E-01	25	K072	1 0 1 1 1	
1.479E-03	1.570E-01	25	K119	1 0 0 0 2	
1.789E-03	1.900E-01	25	L319	1 0 2 1 1	
1.224E-03	1.300E-01	25	M087	1 1 2 1 1	
2.020E-03	2.145E-01	25	M342	1 0 1 1 2	
1.743E-03	1.850E-01	25	P003	2 2 2 2 2	
1.479E-03	1.570E-01	25	P051	2 1 1 2 2	
1.469E-03	1.560E-01	25	S005	2 2 2 2 2	
1.469E-03	1.560E-01	25	S191	1 2 2 2 2	
1.469E-03	1.560E-01	25	S358	2 1 2 2 2	
1.510E-03	1.603E-01	25	S359	2 1 2 2 2	
2.020E-03	2.145E-01	25	W300	2 2 2 2 2	
1.479E-03	1.570E-01	25.00	P007	2 1 2 2 2	
1.589E-03	1.687E-01	29.99	C350	0 0 0 0 0	
1.766E-03	1.875E-01	39.99	C350	0 0 0 0 0	
2.410E-03	2.559E-01	43.0	P005	1 1 2 1 2	
1.911E-03	2.029E-01	49.99	C350	0 0 0 0 0	
2.832E-03	3.007E-01	56.4	P005	1 1 2 1 2	
2.244E-03	2.382E-01	59.99	C350	0 0 0 0 0	
3.199E-03	3.396E-01	65.0	P005	1 1 2 1 2	
2.683E-03	2.848E-01	69.99	C350	0 0 0 0 0	
3.643E-03	3.868E-01	75.3	P005	1 1 2 1 2	
3.171E-03	3.367E-01	79.99	C350	0 0 0 0 0	
4.326E-03	4.593E-01	87.2	P005	1 1 2 1 2	
3.721E-03	3.950E-01	89.99	C350	0 0 0 0 0	
4.853E-03	5.152E-01	99.99	C350	0 0 0 0 0	
2.363E-02	2.509E+00	162.5	P005	1 1 2 1 2	
4.251E-02	4.513E+00	188.1	P005	1 1 2 1 2	
1.614E-01	1.713E+01	243.2	P005	1 1 2 1 2	
4.053E-01	4.303E+01	282.5	P005	1 1 2 1 2	
4.011E-01	4.258E+01	294.9	P005	1 1 2 1 2	
1.743E-03	1.850E-01	ns	H123	0 0 0 0 0	

1498. C_8H_{10}

Xylene
Dimethylbenzene
Xylol

RN: 1330-20-7 **MP** (°C)**:**
MW: 106.17 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-03	8.992E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
1.000E-03	1.062E-01	25	H332	2 2 2 2 0	
<9.41E-03	<9.99E-01	25.50	O005	2 0 2 2 0	
9.419E-03	1.000E+00	150	J023	1 1 2 2 0	
3.297E-02	3.500E+00	200	J023	1 1 2 2 1	
1.036E-01	1.100E+01	250	J023	1 1 2 2 1	

1499. $C_8H_{10}NO_5PS$

Methyl parathion
Parathion-methyl
Methylparathion

RN: 298-00-0 **MP** (°C)**:** 36
MW: 263.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.282E-05	2.180E-02	10	B324	0 0 0 0 0	
8.283E-05	2.180E-02	10	B324	0 0 0 0 0	
1.432E-04	3.770E-02	19.50	B169	2 2 1 1 2	
1.444E-04	3.801E-02	20	B324	0 0 0 0 0	
1.444E-04	3.800E-02	20	B324	0 0 0 0 0	
9.498E-05	2.500E-02	20	M040	1 0 0 1 1	
2.090E-04	5.500E-02	25	M061	1 0 0 0 1	
2.185E-04	5.750E-02	25	M161	1 0 0 0 0	
2.089E-04	5.500E-02	25	Z409	0 0 0 0 0	EFG
2.223E-04	5.851E-02	30	B324	0 0 0 0 0	
2.222E-04	5.850E-02	30	B324	0 0 0 0 0	
1.900E-04	5.000E-02	ns	C117	0 0 0 0 0	
1.445E-04	3.805E-02	ns	R427	0 0 0 0 0	
1.432E-04	3.770E-02	ns	V414	0 0 0 0 0	

1500. $C_8H_{10}N_2O$

p-Phenylenediaminemono-*N*-acetate
p-Phenylendiamin-mono-*N*-acetat

RN: 589-29-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	6.200E+01	57	F300	1 0 0 0 1	

1501. $C_8H_{10}N_2O$
m-Aminoacetanilide
3-Aminoacetanilide
RN: 102-28-3 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.526E-01	8.299E+01	48.7	S115	1 2 1 1 2	
1.021E+00	1.534E+02	82.9	S115	1 2 1 1 2	

1502. $C_8H_{10}N_2O$
o-Aminoacetanilide
2-Aminoacetanilide
RN: 34801-09-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.189E-01	3.288E+01	7.2	S115	1 2 1 1 2	
7.161E-01	1.075E+02	22.0	S115	1 2 1 1 2	
1.215E+00	1.825E+02	33.5	S115	1 2 1 1 2	
1.612E+00	2.421E+02	42.1	S115	1 2 1 1 2	
1.958E+00	2.940E+02	50.4	S115	1 2 1 1 2	
2.270E+00	3.409E+02	59.1	S115	1 2 1 1 2	
2.601E+00	3.906E+02	69.9	S115	1 2 1 1 2	
2.781E+00	4.177E+02	78.2	S115	1 2 1 1 2	
2.943E+00	4.420E+02	88.1	S115	1 2 1 1 2	
3.075E+00	4.618E+02	99.0	S115	1 2 1 1 2	
3.213E+00	4.825E+02	115.4	S115	1 2 1 1 2	

1503. $C_8H_{10}N_2O$
1-(2-Tolyl)urea
o-Tolylurea
RN: 614-77-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-02	2.504E+00	45	W044	1 0 1 0 2	

1504. $C_8H_{10}N_2O$
1-Methyl-3-phenylurea
Desfenuron
N-Phenyl-*N′*-methylurea
Desphenuron
N-Methyl-*N′*-phenylurea
IPO 4328
RN: 1007-36-9 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E+00	7.400E+02	45	W044	1 0 1 0 2	

1505. $C_8H_{10}N_2O$
1-(4-Tolyl)urea
p-Tolylurea
RN: 622-51-5 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.044E-02	3.070E+00	45	W044	1 0 1 0 2	

1506. $C_8H_{10}N_2O$
p-Aminoacetanilide
4-Aminoacetanilide
RN: 122-80-5 **MP** (°C)**:** 164.5
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.061E-01	1.593E+01	25	D044	0 0 0 0 0	
4.064E-01	6.103E+01	56.8	S115	1 2 1 1 2	
1.046E+00	1.570E+02	86.3	S115	1 2 1 1 2	
1.441E+00	2.165E+02	92.1	S115	1 2 1 1 2	
1.699E+00	2.552E+02	93.7	S115	1 2 1 1 2	
1.996E+00	2.998E+02	96.5	S115	1 2 1 1 2	
2.193E+00	3.293E+02	98.6	S115	1 2 1 1 2	

1507. $C_8H_{10}N_2O$
Methylbenzylnitrosamine
N-Nitroso(methyl)benzylamine
N-Nitroso-*N*-methylbenzylamine
N-Nitroso(benzyl)methylamine
N-Nitroso-*N*-methylbenzenemethanamine
RN: 937-40-6 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	4.505E+00	24	D083	2 0 0 0 1	

1508. $C_8H_{10}N_2O$
Benzylurea
Benzyl-harnstoff
RN: 538-32-9 **MP** (°C)**:** 147
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-01	1.700E+01	45	F300	1 0 0 0 2	
1.139E-01	1.710E+01	45	W044	1 0 1 0 2	

1509. $C_8H_{10}N_2O_3$
5-Methyl-5-allylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(2-propenyl)
5-Methyl-5-allylbarbiturate
RN: 143585-01-7 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-02	1.261E+01	25	P350	0 0 0 0 0	intrinsic

1510. $C_8H_{10}N_2O_3$
5,5-Tetramethylenebarbituric acid
7,9-Diazaspiro[4.5]decane-6,8,10-trione
Spirocyclopentabarbituric acid
Cyclopentane-spirobarbiturate
RN: 56209-30-4 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.476E-03	8.154E-01	25	P350	0 0 0 0 0	intrinsic

1511. $C_8H_{10}N_2O_3S$
*N*1-Acetylsulfanilamide
Sulfacetamide
Acetyl sulfacetamide
RN: 144-80-9 **MP** (°C)**:** 183
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.881E-02	1.260E+01	20	F073	1 2 2 2 2	
3.871E-02	8.293E+00	25	M440	0 0 0 0 0	
5.834E-03	1.250E+00	37	B046	1 0 2 2 2	pH 4.5
5.834E-02	1.250E+01	37	B046	1 0 2 2 2	pH 5
6.908E-02	1.480E+01	37	D084	1 0 1 0 2	
5.601E-02	1.200E+01	37	K086	1 0 0 0 2	
5.134E-02	1.100E+01	37	L091	1 0 0 0 2	pH 5.5
2.327E-02	4.985E+00	ns	L044	0 0 0 0 2	
3.090E-02	6.621E+00	ns	R427	0 0 0 0 0	

1512. $C_8H_{10}N_2O_3S$
*N*4-Acetylsulfanilamide
*N*4-Acetylsulphanilamide
RN: 121-61-9 **MP** (°C)**:** 216
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.474E-02	5.300E+00	37	L091	1 0 0 0 2	pH 5.5
2.479E-02	5.312E+00	37.50	M142	1 0 0 0 2	

1513. $C_8H_{10}N_2O_3S$
Tosylurea
Tosyluree
RN: 1694-06-0 **MP** (°C)**:**
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.631E-03	7.779E-01	37	A028	1 0 2 1 2	intrinsic

1514. $C_8H_{10}N_2O_4S$

Asulam

Methyl *N*-(4-aminobenzenesulphonyl)carbamate

RN: 3337-71-1 **MP** (°C)**:** 144

MW: 230.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-02	4.975E+00	ns	M061	0 0 0 0 0	
2.188E-02	5.037E+00	ns	R427	0 0 0 0 0	
2.172E-02	5.000E+00	rt	M161	0 0 0 0 0	

1515. $C_8H_{10}N_4O_2$

Caffeine

Coffein

RN: 58-08-2 **MP** (°C)**:** 238

MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-02	7.548E+00	0	H023	1 0 2 1 2	
3.800E-02	7.379E+00	1	M116	2 1 1 1 1	
3.757E-02	7.296E+00	2	C074	1 0 0 1 2	
4.786E+00	9.294E+02	5	B429	1 0 1 2 2	
4.859E+00	9.436E+02	15	B429	1 0 1 2 2	
6.603E-02	1.282E+01	15	H023	1 0 2 1 2	
5.800E-02	1.126E+01	15	O017	1 0 1 1 1	
5.770E-02	1.121E+01	15	O018	1 2 1 1 2	
5.770E-02	1.121E+01	15	O019	1 0 0 1 2	
6.859E-02	1.332E+01	16	A072	1 0 1 0 2	
7.415E-02	1.440E+01	20	F300	1 0 0 0 2	
6.779E-02	1.316E+01	20	J009	2 0 2 2 2	
1.242E-01	2.411E+01	25	A068	2 0 0 0 2	
4.931E+00	9.575E+02	25	B429	1 0 1 2 2	
1.066E-01	2.071E+01	25	E016	1 1 1 1 2	
1.081E-01	2.100E+01	25	F300	1 0 0 0 1	
1.080E-01	2.097E+01	25	L329	2 2 1 2 2	
1.110E-01	2.156E+01	25	M116	2 1 1 1 2	
1.244E-01	2.415E+01	25	M158	2 0 2 2 2	
1.000E-01	1.942E+01	25	O017	1 0 1 1 2	
1.002E-01	1.946E+01	25	O018	1 2 1 1 2	
1.098E-02	2.132E+00	25	O019	1 0 0 1 2	
1.272E-01	2.470E+01	25	O302	1 0 0 1 0	
1.107E-01	2.150E+01	25	P010	1 0 1 1 2	
1.123E-01	2.180E+01	25	P011	0 0 0 0 0	
1.195E-01	2.320E+01	25	P018	1 0 2 2 2	
1.081E-01	2.100E+01	25	P020	2 0 1 1 1	
1.330E-01	2.583E+01	30	B042	1 2 1 1 2	
1.330E-01	2.583E+01	30	G021	1 0 0 0 2	
1.330E-01	2.583E+01	30	H020	1 0 0 0 2	
1.333E-01	2.589E+01	30	H023	1 0 2 1 2	

(*continued*)

1515. $C_8H_{10}N_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	2.583E+01	30.60	M116	2 1 1 1 2	
4.999E+00	9.707E+02	35	B429	1 0 1 2 2	
1.670E-01	3.243E+01	35	O017	1 0 1 1 2	
1.909E-01	3.707E+01	37	C074	1 0 0 1 2	
1.930E-01	3.748E+01	37	M116	2 1 1 1 2	
5.041E+00	9.789E+02	40	B429	1 0 1 2 2	
2.266E-01	4.400E+01	40	F300	1 0 0 0 1	
5.211E-01	1.012E+02	57	C074	1 0 0 1 2	
1.408E+00	2.735E+02	83	C065	1 0 0 1 2	
1.407E+00	2.733E+02	85	C074	1 0 0 1 2	
1.739E+00	3.377E+02	87	C065	1 0 0 1 2	
2.343E+00	4.550E+02	90	C074	1 0 0 1 2	
1.287E-01	2.500E+01	ns	D035	0 0 0 0 2	
1.104E-01	2.143E+01	rt	D021	0 0 1 1 2	
1.596E-04	3.100E-02	rt	N015	0 0 2 2 1	*sic*
4.892E-02	9.500E+00	rt	R431	0 0 0 0 0	Average

1516. $C_8H_{10}N_4O_2.H_2O$

Caffeine (monohydrate)

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-, monohydrate

RN: 5743-12-4 **MP** (°C)**:** 178

MW: 212.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-01	2.146E+01	25	D004	0 0 0 0 0	

1517. $C_8H_{10}N_4O_3$

1,3,7-Trimethyluric acid

8-Oxy-caffeine

RN: 5415-44-1 **MP** (°C)**:** 374

MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	2.400E-02	rt	N015	0 0 2 2 1	

1518. $C_8H_{10}O$
4-Ethylphenol
p-Ethylphenol
RN: 123-07-9 **MP** (°C)**:** 43.5
MW: 122.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.854E-02	5.931E+00	20	R087	0 0 0 0 0	0.15M NaCl
2.332E-02	2.849E+00	25	L022	1 0 0 0 0	
4.011E-02	4.900E+00	25	M127	1 0 0 0 1	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
4.467E-02	5.457E+00	ns	R427	0 0 0 0 0	

1519. $C_8H_{10}O$
2,3-Xylenol
2,3-Dimethylphenol
RN: 526-75-0 **MP** (°C)**:** 75
MW: 122.17 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.740E-02	4.569E+00	25	A021	1 2 1 1 2	

1520. $C_8H_{10}O$
Phenylethylalcohol
Phenyl ethyl alcohol
RN: 60-12-8 **MP** (°C)**:**
MW: 122.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-01	1.796E+01	20	S006	1 0 0 0 2	
1.720E-01	2.101E+01	25	D407	1 0 2 2 2	
1.432E-01	1.749E+01	25	H044	1 0 2 1 2	
1.455E-01	1.778E+01	30	H044	1 0 2 1 2	
1.487E-01	1.816E+01	35	H044	1 0 2 1 2	
1.518E-01	1.855E+01	40	H044	1 0 2 1 2	
1.542E-01	1.884E+01	45	H044	1 0 2 1 2	
1.562E-01	1.908E+01	50	H044	1 0 2 1 2	
1.597E-01	1.951E+01	55	H044	1 0 2 1 2	

1521. $C_8H_{10}O$
Phloral
RN: **MP** (°C)**:**
MW: 122.17 **BP** (°C)**:** 204.52

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-02	4.975E+00	25	L022	1 0 0 0 0	

1522. $C_8H_{10}O$
2,6-Xylenol
1,3,2-Xylenol
2,6-Dimethylphenol
Vic-*m*-xylenol
RN: 576-26-1 **MP** (°C)**:** 49
MW: 122.17 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-02	4.392E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.950E-02	6.047E+00	25	A021	1 2 1 1 2	
5.100E-02	6.231E+00	25	B316	0 0 0 0 0	

1523. $C_8H_{10}O$
2,4-Xylenol
2,4-Dimethylphenol
m-Xylenol
2,4-Dimethyl-phenol-
Phenol, 2,4-dimethyl-
1-Hydroxy-2,4-dimethylbenzene
RN: 105-67-9 **MP** (°C)**:** 26
MW: 122.17 **BP** (°C)**:** 211.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-02	5.375E+00	20	K132	1 0 1 1 1	
4.300E-02	5.253E+00	20	K309	1 0 0 1 1	
5.271E-02	6.440E+00	20	R087	0 0 0 0 0	0.15M NaCl
5.100E-02	6.231E+00	25	A021	1 2 1 1 2	
6.440E-02	7.868E+00	25	B173	2 0 2 2 2	
7.200E-02	8.796E+00	25	B316	0 0 0 0 0	
6.499E-02	7.940E+00	25	M127	1 0 0 0 2	
2.190E-01	2.675E+01	80	K309	1 0 0 1 2	

1524. $C_8H_{10}O$
α-Methyl-benzenemethanol
α-Methylbenzyl alcohol
1-Phenylethan-1-*o*
Methylphenylcarbinol
β-Hydroxyethylbenzene
(*S*)-1-Phenylethyl alcohol
RN: 98-85-1 **MP** (°C)**:** 20
MW: 122.17 **BP** (°C)**:** 401 at 0 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E+00	8.427E+02	14.57	L441	0 0 0 0 0	
6.860E+00	8.380E+02	19.84	L441	0 0 0 0 0	

(*continued*)

1524. $C_8H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.056E-01	6.177E+01	92.71	L441	0 0 0 0 0	
6.491E+00	7.930E+02	94.89	L441	0 0 0 0 0	
6.445E+00	7.874E+02	105.95	L441	0 0 0 0 0	
6.196E+00	7.569E+02	127.92	L441	0 0 0 0 0	

1525. $C_8H_{10}O$

Phenetole
Ethoxybenzene

RN: 103-73-1 **MP** (°C)**:** –30
MW: 122.17 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	5.498E-01	25	M327	1 0 0 1 2	
4.657E-03	5.690E-01	25.04	V013	2 2 2 2 2	

1526. $C_8H_{10}O$

2,5-Xylenol
2,5-Dimethylphenol
p-Xylenol
2,5-Dimethyl-phenol-
Phenol, 2,5-dimethyl-

RN: 95-87-4 **MP** (°C)**:** 75
MW: 122.17 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	3.543E+00	25	A021	1 2 1 1 2	
2.600E-02	3.176E+00	25	B316	0 0 0 0 0	

1527. $C_8H_{10}O$

4-Methylbenzyl alcohol
4-Methyl-benzylalkohol

RN: 589-18-4 **MP** (°C)**:** 60
MW: 122.17 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-02	8.430E+00	20	B407	1 0 1 2 2	

1528. $C_8H_{10}O$
3,4-Xylenol
3,4-Dimethylphenol
As-*o*-xylenol
RN: 95-65-8 **MP** (°C)**:** 62.5
MW: 122.17 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	3.787E+00	20	K132	1 0 1 1 1	
3.900E-02	4.765E+00	25	A021	1 2 1 1 2	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
2.530E-02	3.091E+00	37	E028	1 0 1 1 2	

1529. $C_8H_{10}O$
3,5-Xylenol
3,5-Dimethylphenol
RN: 108-68-9 **MP** (°C)**:** 64
MW: 122.17 **BP** (°C)**:** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-02	4.032E+00	20	K132	1 0 1 1 1	
2.961E-02	3.618E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.000E-02	4.887E+00	25	A021	1 2 1 1 2	
4.000E-02	4.887E+00	25	B316	0 0 0 0 0	
3.981E-02	4.864E+00	ns	R427	0 0 0 0 0	

1530. $C_8H_{10}O_2$
o-Ethoxyphenol
2-Ethoxyphenol
RN: 94-71-3 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-02	8.414E+00	24.99	B353	0 0 0 0 0	

1531. $C_8H_{10}O_2$
Veratrole
o-Dimethoxybenzene
RN: 91-16-7 **MP** (°C)**:** 15
MW: 138.17 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.842E-02	6.690E+00	25	L348	1 2 2 1 2	

1532. $C_8H_{10}O_2$
1,3-Dimethoxybenzene
m-Dimethoxybenzene
Dimethylresorcinol
RN: 151-10-0 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:** 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.800E-03	1.216E+00	25	M327	1 0 0 1 2	

1533. $C_8H_{10}O_2$
2-Phenoxyethanol
Phenoxyethyl alcohol
Ethylene glycol phenyl ether
Arosol
1-Hydroxy-2-phenoxyethane
Phenoxethol
RN: 122-99-6 **MP** (°C)**:** 12
MW: 138.17 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.882E-01	2.601E+01	20	M062	1 0 0 0 2	
2.610E-01	3.606E+01	37	E028	1 0 1 1 2	

1534. $C_8H_{10}O_2$
3-Ethoxyphenol
m-Ethoxy phenol
Resorcinol monoethyl ether
RN: 621-34-1 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.382E+01	25	B314	0 0 0 0 0	
1.003E-01	1.386E+01	30	B315	0 0 0 0 0	

1535. $C_8H_{10}O_2$
p-Ethoxyphenol
Hydroquinone monoethyl ether
RN: 622-62-8 **MP** (°C)**:** 64.5–67.5
MW: 138.17 **BP** (°C)**:** 131 at 9 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.097E-02	7.043E+00	20	R087	0 0 0 0 0	0.15M NaCl

1536. $C_8H_{10}O_2$
p-Dimethoxybenzene
4-Dimethoxybenzene
RN: 150-78-7 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-05	7.641E-03	25	C316	0 0 0 0 0	0.1M NaCl

1537. $C_8H_{10}O_3$
1,3-Dimethyl ether pyrogallol
Pyrogallol-1,3-dimethylaether
2,6-Dimethoxyphenol
RN: 91-10-1 **MP** (°C)**:** 56
MW: 154.17 **BP** (°C)**:** 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.116E-01	1.720E+01	13	F300	1 0 0 0 2	

1538. $C_8H_{10}O_3S$
Benzene sulfonic acid ethyl ester
Ethyl benzenesulfonate
Ethyl phenylsulfonate
RN: 515-46-8 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.390E-03	1.376E+00	25	K097	2 0 2 2 2	

1539. $C_8H_{10}O_4$
Cyclohexene-1,4-dicarboxylic acid
Cyclohexen-(1)-dicarbonsaeure-(1,4)
RN: 2205-27-8 **MP** (°C)**:** 312
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-03	2.000E-01	20	F300	1 0 0 0 0	

1540. $C_8H_{10}O_4$
2-Cyclohexene-1,2-dicarboxylic acid
Cyclohexen-(2)-dicarbonsaeure-(1,2)
RN: 38765-78-5 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.113E-02	8.700E+00	10	F300	1 0 0 0 1	

1541. $C_8H_{10}O_5$
Endothall
Endothal
RN: 145-73-3 **MP** (°C)**:** 144
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.883E-01	9.091E+01	20	B200	1 0 0 0 2	
5.372E-01	1.000E+02	20	M161	1 0 0 0 2	
4.883E-01	9.091E+01	ns	B100	0 0 0 0 0	
4.883E-01	9.091E+01	ns	C307	0 0 0 0 1	

1542. $C_8H_{10}O_8$
meso-1,2,3,4-Butanetetracarboxylic acid
1,2,3,4-Butanetetracarboxylic acid
Butanetetracarboxylic acid
1,2,3,4,-Butane tetracarboxylic acid
RN: 1703-58-8 **MP** (°C)**:** 196
MW: 234.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.606E-01	1.547E+02	25	M370	1 2 2 1 2	

1543. $C_8H_{11}BrN_2O_2$
Isocil
Uracil, 5-bromo-3-isopropyl-6-methyl-
RN: 314-42-1 **MP** (°C)**:** 158–159
MW: 247.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.701E-03	2.150E+00	25	B185	0 0 0 0 0	

1544. $C_8H_{11}Cl_2NO$
N,N-Diallyldichloroacetamide
Dichlormid
N,N-Diallyl dichloroacetamide
2,2-Dichloro-*N,N*-di-2-propenylacetamide
R 25788
RN: 37764-25-3 **MP** (°C)**:** 5
MW: 208.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.403E-02	5.000E+00	20	M161	1 0 0 0 0	
2.399E-02	4.992E+00	ns	S460	0 0 0 0 0	

1545. $C_8H_{11}Cl_3O_6$
Chloralose
1,2-*O*-(2,2,2-Trichloroethylidene)-α-D-glucofuranose
Anhydroglucochloral
Alfamat
Aphosal
Murex
RN: 15879-93-3 **MP** (°C)**:** 187
MW: 309.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-02	4.440E+00	15	M161	1 0 0 0 2	

1546. $C_8H_{11}N$
Xylidine
N,N-Dimethylaniline
Dimethylaminobenzene
Benzenamine
Aminodimethylbenzene
RN: 121-69-7 **MP** (°C)**:** 2
MW: 121.18 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.120E-03	1.105E+00	25	C113	1 0 2 1 2	

1547. $C_8H_{11}NO$
Tyramine
Tyramin
4-Hydroxyphenylethylamine
4-(2-Aminoethyl)phenol
2-(*p*-Hydroxyphenyl)ethylamine
RN: 51-67-2 **MP** (°C)**:** 164.5
MW: 137.18 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.574E-02	1.039E+01	15	D041	1 0 0 0 2	
7.581E-02	1.040E+01	15	F300	1 0 0 0 2	

1548. $C_8H_{11}NO$
Phenylethanolamine
Phenyl ethanolamine
2-Anilinoethanol
β-Hydroxyethyl aniline
N-Phenylethanolamine
PEA
RN: 7568-93-6 **MP** (°C)**:** 56.5
MW: 137.18 **BP** (°C)**:** 286.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.192E-01	4.379E+01	20	M062	1 0 0 0 2	

1549. $C_8H_{11}N_2O_5PS$
Parathion-amino
Aminoparathion
RN: **MP** (°C)**:**
MW: 278.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.419E-03	3.948E-01	19.50	B169	2 2 1 1 2	

1550. $C_8H_{11}N_3O_3S$
Lamivudine
2(1H)-Pyrimidinone,4-amino-1-[2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-,(2R-*cis*)
Epivir
3′-Thia-2′,3′-dideoxcytidine
(–)NGPB-21
(–) 2′-Deoxy-3′-thiacytidine
RN: 134678-17-4 **MP** (°C)**:**
MW: 229.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-01	7.000E+01	ns	K444	0 0 0 0 0	
3.053E-01	7.000E+01	rt	B435	0 0 0 0 0	

1551. $C_8H_{11}N_5O_3$
Acyclovir
Acycloguanosine
9-(2-Hydroxyethoxymethyl)guanine
6H-Purin-6-one, 2-amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]-
Cargosil
Zovirax
RN: 59277-89-3 **MP** (°C)**:**
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.216E-03	1.400E+00	21	B419	1 1 2 2 1	int
7.150E-03	1.610E+00	22	K443	0 0 0 0 0	
7.244E-03	1.631E+00	22	K445	0 0 0 0 0	
5.380E-03	1.212E+00	22.5	B422	2 0 2 2 2	
2.240E+00	5.045E+02	25	B443	0 0 0 0 0	
8.070E-03	1.817E+00	25	Z407	0 0 0 0 0	
4.440E-02	1.000E+01	ns	K444	0 0 0 0 0	
6.166E-03	1.389E+00	ns	R427	0 0 0 0 0	

1552. C_8H_{12}
4-Vinylcyclohexene
4-Vinyl-1-cyclohexene
RN: 100-40-3 **MP** (°C)**:** –101
MW: 108.18 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.622E-04	5.000E-02	25	M001	2 1 2 2 1	

1553. $C_8H_{12}ClNO$
Allidochlor
CDAA
N,N-Diallyl-2-chloroacetamide
Randox
2-Chloro-*N,N*-diallylacetamide
CP 6343
RN: 93-71-0 **MP** (°C)**:**
MW: 173.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.113E-01	1.932E+01	22	J008	1 0 0 0 2	
1.113E-01	1.932E+01	25	B185	0 0 0 0 0	
1.135E-01	1.970E+01	25	G319	0 0 0 0 0	
1.135E-01	1.970E+01	25	M161	1 0 0 0 2	
1.129E-01	1.961E+01	ns	B100	0 0 0 0 0	
1.130E-01	1.962E+01	ns	F184	0 0 0 0 2	
1.129E-01	1.961E+01	ns	M061	0 0 0 0 0	
3.162E-01	5.491E+01	ns	M163	0 0 0 0 0	EFG

1554. $C_8H_{12}N_2O_2S$

*N*1-Dimethylsulfanilamide
p-Amino-*N,N*-dimethylbenzenesulfonamide
[(4-Aminophenyl)sulfonyl]dimethylamine
p-(Dimethylsulfamoyl)aniline

RN: 1709-59-7 **MP** (°C)**:**
MW: 200.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	6.268E-01	37	K095	2 0 0 0 2	intrinsic

1555. $C_8H_{12}N_2O_2S$

5,5-Diethyl-2-thiobarbituric acid
4,6(1H,5H)-Pyrimidinedione, 5,5-diethyldihydro-2-thioxo
Barbituric acid, 5,5-diethyl-2-thio
Certodorm

RN: 77-32-7 **MP** (°C)**:**
MW: 200.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.810E-03	1.364E+00	25	P350	0 0 0 0 0	intrinsic

1556. $C_8H_{12}N_2O_3$

Barbital
5,5-Diethylbarbituric acid
Diethylmalonylurea

RN: 57-44-3 **MP** (°C)**:** 190
MW: 184.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.131E+00	0	M143	1 2 1 1 0	
1.900E-02	3.500E+00	0	M143	1 2 1 1 2	
2.562E-02	4.720E+00	10	N007	1 2 2 2 2	form I
1.900E-02	3.500E+00	10	N007	1 2 2 2 2	form III
3.100E-02	5.710E+00	14	I006	1 0 0 0 1	
3.187E-02	5.870E+00	15	H018	0 0 0 0 0	
3.500E-02	6.447E+00	19	I006	1 0 0 0 1	
4.522E-02	8.330E+00	20	D041	1 0 0 0 1	
3.637E-02	6.700E+00	20	F300	1 0 0 0 1	
3.415E-02	6.290E+00	20	J030	1 2 2 2 2	
2.839E-02	5.230E+00	20	N007	1 2 2 2 2	form III
3.409E-02	6.280E+00	20	N007	1 2 2 2 2	form I
3.806E-02	7.011E+00	20	S146	2 2 2 1 2	form I
3.752E-02	6.912E+00	20	S146	2 2 2 1 2	form II
3.881E-02	7.149E+00	25	A023	1 0 0 1 2	
3.963E-02	7.300E+00	25	B011	2 0 0 1 0	
3.971E-02	7.314E+00	25	B065	1 1 1 1 1	
3.746E-02	6.900E+00	25	B167	1 1 0 0 1	pH 5.7

(*continued*)

1556. $C_8H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-02	7.110E+00	25	G003	1 1 1 1 2	pH 4.7
2.800E-02	5.158E+00	25	M143	1 2 1 1 2	
4.050E-02	7.460E+00	25	M310	2 2 2 2 2	
4.018E-02	7.401E+00	25	P350	0 0 0 0 0	intrinsic
4.239E-02	7.809E+00	25	S146	2 2 2 1 2	form II
4.010E-03	7.386E-01	25	V033	2 0 1 1 2	
4.010E-02	7.386E+00	25.00	T303	1 0 0 0 2	
4.300E-02	7.920E+00	27	I006	1 0 0 0 1	
4.300E-02	7.920E+00	30	G014	1 1 1 1 0	EFG, 0.003N H_2SO_4
2.704E-02	4.980E+00	30	H005	1 0 1 2 2	average of 4
4.408E-02	8.119E+00	30	H018	0 0 0 0 0	
4.400E-02	8.105E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
4.260E-02	7.847E+00	30	K108	1 2 2 0 2	
4.425E-02	8.150E+00	30	N007	1 2 2 2 2	form I
4.207E-02	7.750E+00	30	N007	1 2 2 2 2	form III
4.720E-02	8.694E+00	30	S146	2 2 2 1 2	form I
4.618E-02	8.507E+00	30	S146	2 2 2 1 2	form II
5.162E-02	9.509E+00	35	S146	2 2 2 1 2	form I
5.184E-02	9.548E+00	35	S146	2 2 2 1 2	form II
5.150E-02	9.486E+00	35.00	T303	1 0 0 0 2	
4.843E-02	8.920E+00	36	A023	1 0 0 1 2	
5.152E-02	9.490E+00	37	J030	1 2 2 2 2	
5.300E-02	9.762E+00	37	K121	1 2 1 2 1	0.1N HCl
5.538E-02	1.020E+01	37	N007	1 2 2 2 2	form III
5.277E-02	9.720E+00	37	N007	1 2 2 2 2	form I
5.668E-02	1.044E+01	37	S146	2 2 2 1 2	form II
5.588E-02	1.029E+01	40	A023	1 0 0 1 1	
6.100E-01	1.124E+02	40	N008	1 0 1 1 2	*sic*
6.967E-02	1.283E+01	45	S146	2 2 2 1 2	form II
6.800E-02	1.253E+01	45.00	T303	1 0 0 0 2	
4.343E-01	8.000E+01	100	F300	1 0 0 0 1	
3.257E-02	6.000E+00	ns	T003	0 0 0 0 2	

1557. $C_8H_{12}O_2$

1-Epoxyethyl-3,4-epoxycyclohexane
Vinylcyclohexene dioxide

RN: 106-87-6 **MP** (°C)**:** <–55
MW: 140.18 **BP** (°C)**:** 227

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E+00	1.547E+02	20	I313	0 0 0 0 0	

1558. $C_8H_{12}O_4$
trans-Cyclohexane-1,2-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,2)
RN: 2305-32-0 **MP** (°C)**:**
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-02	2.000E+00	20	F300	1 0 0 0 0	

1559. $C_8H_{12}O_4$
cis-Cyclohexane-1,2-dicarboxylic acid
cis-Cyclohexan-dicarbonsaeure-(1,2)
RN: 610-09-3 **MP** (°C)**:** 193
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.16E-02	>2.00E+00	20	F300	1 0 0 0 0	

1560. $C_8H_{12}O_4$
trans-Cyclohexane-1,4-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,4)
RN: 619-82-9 **MP** (°C)**:**
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.646E-03	8.000E-01	17	F300	1 0 0 0 0	
7.550E-02	1.300E+01	100	F300	1 0 0 0 1	

1561. $C_8H_{13}BrN_2O_2$
α-Bromethylpropylaceturea
RN: **MP** (°C)**:**
MW: 249.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-03	4.098E-01	20	O021	1 0 0 0 0	

1562. $C_8H_{13}NO$
Diaalylacetamide
α,α-Diallylacetamide
2-(2-Propenyl)4-pentenamide
RN: 60730-94-1 **MP** (°C)**:**
MW: 139.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.750E+01	ns	H348	0 0 0 0 0	

1563. $C_8H_{13}N_2O_3PS$
Thionazin
O,O-Diethyl *O*-pyrazinyl thiophosphate
RN: 297-97-2 **MP** (°C)**:** –1.7
MW: 248.24 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.140E+00	25	M061	1 0 0 0 2	
4.592E-03	1.140E+00	27	M161	1 0 0 0 2	

1564. C_8H_{14}
1-Octyne
Hexylacetylene
n-Hexylacetylene
RN: 629-05-0 **MP** (°C)**:** –80
MW: 110.20 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.178E-04	2.400E-02	25	M001	2 1 2 2 2	

1565. C_8H_{14}
2,2-Dimethyl-3-hexyne
1-Ethyl-2-tertbutylacetylene
RN: 4911-60-8 **MP** (°C)**:**
MW: 110.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	7.934E-02	25	H039	1 2 2 2 1	

1566. $C_8H_{14}ClNS_2$
Carbamic acid, diethyldithio-2chloroallyl ester
2-Chloroallyl diethyldithiocarbamate
CDEC
RN: 95-06-7 **MP** (°C)**:** <25
MW: 223.79 **BP** (°C)**:** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.469E-04	1.000E-01	25	B185	0 0 0 0 0	
4.111E-04	9.200E-02	25	B200	1 0 0 0 1	
4.469E-04	1.000E-01	25	F019	1 0 0 0 2	
4.111E-04	9.200E-02	25	G319	0 0 0 0 0	
4.111E-04	9.200E-02	25	M161	1 0 0 0 1	
4.468E-04	9.999E-02	ns	M061	0 0 0 0 0	approximate

1567. $C_8H_{14}ClN_5$
Atrazine
2-Chloro-4-ethylamino-6-isopropylamino-*s*-triazine
RN: 1912-24-9 **MP** (°C)**:** 172
MW: 215.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-04	2.200E-02	0	B185	0 0 0 0 0	
1.390E-04	2.998E-02	1	G091	1 0 1 2 2	pH 6.0
5.000E-04	1.078E-01	2	B193	1 2 0 0 0	
1.410E-04	3.041E-02	8	G091	1 0 1 2 2	pH 6.0
1.530E-04	3.300E-02	20	A314	0 0 0 0 0	
1.345E-04	2.900E-02	20	C048	2 2 2 2 1	
1.391E-04	3.000E-02	20	E048	1 2 1 1 1	
1.391E-04	3.000E-02	20	F311	1 2 2 2 1	
1.580E-04	3.408E-02	20	G091	1 0 1 2 2	pH 6.0
1.298E-04	2.800E-02	20	M161	1 0 0 0 1	
1.391E-04	3.000E-02	20	N333	0 0 0 0 0	
3.245E-04	7.000E-02	21	B192	0 0 0 0 1	
3.245E-04	7.000E-02	21	G099	2 0 0 1 0	
3.245E-04	7.000E-02	22	M061	1 0 0 0 1	
1.530E-04	3.300E-02	25	H024	2 2 2 2 2	
1.386E-04	2.990E-02	25	H073	2 1 1 2 2	
1.530E-04	3.300E-02	25	P434	0 0 0 0 0	
3.245E-04	7.000E-02	27	B185	0 0 0 0 0	
1.530E-04	3.300E-02	27	B200	1 0 0 0 1	
1.970E-04	4.249E-02	29	G091	1 0 1 2 2	pH 6.0
4.530E-04	9.771E-02	50	G001	1 0 0 1 2	
1.484E-03	3.200E-01	85	B185	0 0 0 0 0	
3.245E-04	7.000E-02	ns	C101	0 0 0 0 1	
3.245E-04	7.000E-02	ns	G041	0 0 0 0 1	
3.245E-04	7.000E-02	ns	H112	0 0 0 0 1	
1.530E-04	3.300E-02	ns	J033	0 0 0 0 0	
3.941E-04	8.500E-02	ns	M110	0 0 0 0 0	EFG
1.609E-04	3.470E-02	ns	V414	0 0 0 0 0	

1568. $C_8H_{14}N_2O_2$
cis-N,N,N′,N′-Tetramethylfumaramide
2-Butenediamide, *N,N,N′,N′*-tetramethyl-, (Z)-
RN: 35075-35-5 **MP** (°C)**:**
MW: 170.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E+00	2.945E+02	30	K019	1 0 0 0 2	

1569. $C_8H_{14}N_4OS$
Metribuzin
4-Amino-6-*tert*-butyl-3-(methylthio)-as-triazin-5(4H)-one
Bayer 6159H
Lexone
Sencor
Sencorex
RN: 21087-64-9 **MP** (°C)**:** 125.8
MW: 214.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	1.200E+00	20	M161	1 0 0 0 1	
5.693E-03	1.220E+00	22.5	G301	0 0 0 0 0	
4.662E-03	9.990E-01	ns	B100	0 0 0 0 0	
7.000E-03	1.500E+00	ns	M110	0 0 0 0 0	EFG

1570. $C_8H_{14}O$
Bicyclo[2.2.1]heptylcarbinol
2-Norcamphanemethanol
RN: 5240-72-2 **MP** (°C)**:**
MW: 126.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.916E-03	9.990E-01	ns	M061	0 0 0 0 0	

1571. $C_8H_{14}O_2$
2,4-Octadione
Valerylacetone
RN: 14090-87-0 **MP** (°C)**:**
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.925E+00	25	M078	2 0 1 0 2	

1572. $C_8H_{14}O_2$
Cyclohexanol acetate
Hexalin acetate
Cyclohexyl acetate
RN: 622-45-7 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.597E+00	20	D052	1 1 0 0 1	
2.033E-02	2.892E+00	23.50	O005	2 0 2 2 1	
2.138E-02	3.040E+00	ns	S460	0 0 0 0 0	

1573. $C_8H_{14}O_2$
6-Methyl-2,4-heptadione
2-Methyl-4,6-heptanedione
Isovalerylacetone
RN: 3002-23-1 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.490E-02	3.541E+00	25	M078	2 0 1 0 2	

1574. $C_8H_{14}O_2$
3-Propyl-2,4-pentadione
3-Acetyl-2-hexanone
RN: 1540-35-8 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	1.891E+01	25	M078	2 0 1 0 2	

1575. $C_8H_{14}O_2$
5,5-Dimethyl-2,4-hexadione
Pivaloylacetone
Pivaloylacetylmethane
RN: 7307-04-2 **MP** (°C)**:**
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-02	3.327E+00	25	M078	2 0 1 0 2	

1576. $C_8H_{14}O_2S_4$
Propyl dixanthogen
bis(1-Propyl) dixanthogen
Propyl xanthogen disulfide
Dipropyl dixanthogen
Dipropyl thioperoxydicarbonate
Dipropyl xanthogen disulfide
RN: 3750-28-5 **MP** (°C)**:**
MW: 270.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.057E-04	25	H102	1 2 1 2 1	

1577. $C_8H_{14}O_4$
Suberic acid
Korksaeure
RN: 505-48-6 **MP** (°C)**:** 142
MW: 174.20 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	8.000E-01	0	L041	1 0 0 1 0	
5.301E-03	9.234E-01	6.99	A340	0 0 0 0 0	
7.097E-03	1.236E+00	12.69	A340	0 0 0 0 0	
8.037E-03	1.400E+00	15	F300	1 0 0 0 1	
7.463E-03	1.300E+00	15	L041	1 0 0 1 1	
7.463E-03	1.300E+00	15	M051	1 0 0 0 1	
9.789E-03	1.705E+00	18.69	A340	0 0 0 0 0	
9.185E-03	1.600E+00	20	L041	1 0 0 1 1	
8.986E-03	1.565E+00	20	M171	1 0 0 0 0	
1.206E-01	2.100E+01	21	B040	1 0 1 1 2	*sic*
1.388E-02	2.417E+00	24.99	A340	0 0 0 0 0	
3.387E-02	5.900E+00	25	F300	1 0 0 0 1	
6.800E-02	1.185E+01	25	K040	1 0 2 1 2	*sic*
1.700E-02	2.961E+00	30	H021	1 0 1 1 0	EFG
1.890E-02	3.293E+00	32.49	A340	0 0 0 0 0	
2.045E-02	3.563E+00	34.49	A340	0 0 0 0 0	
2.583E-02	4.500E+00	35	L041	1 0 0 1 1	
2.326E-02	4.051E+00	39.99	A340	0 0 0 0 0	
2.682E-02	4.673E+00	44.49	A340	0 0 0 0 0	
5.626E-02	9.800E+00	50	L041	1 0 0 1 1	
3.198E-02	5.571E+00	50.19	A340	0 0 0 0 0	
3.534E-02	6.156E+00	52.69	A340	0 0 0 0 0	
5.551E-02	9.670E+00	61.49	A340	0 0 0 0 0	
6.422E-02	1.119E+01	63.99	A340	0 0 0 0 0	
1.274E-01	2.220E+01	65	L041	1 0 0 1 2	
8.182E-02	1.425E+01	70.09	A340	0 0 0 0 0	
1.156E-01	2.013E+01	76.49	A340	0 0 0 0 0	
1.386E-02	2.414E+00	rt	H431	0 0 0 0 0	

1578. $C_8H_{14}O_4$
Diethyl succinate
Butanedioic acid, diethyl ester
RN: 123-25-1 **MP** (°C)**:** –20
MW: 174.20 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.089E-02	1.896E+00	ns	F014	0 0 0 0 2	

1579. $C_8H_{14}O_4$
Butylene glycol diacetate
1,4-Diacetoxybutane
Tetramethylene acetate
RN: 628-67-1 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.005E-01	3.494E+01	26	O012	1 2 1 1 2	
1.602E-01	2.790E+01	50	O012	1 2 1 1 2	
2.048E-01	3.568E+01	75	O012	1 2 1 1 2	

1580. $C_8H_{14}O_4$
Tetramethyl succinic acid
Tetramethyl-bernsteinsaeure
RN: 630-51-3 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.755E-02	4.800E+00	13.5	F300	1 0 0 0 1	

1581. $C_8H_{14}O_4$
Isoamylmalonic acid
Acide isoamylmalonique
RN: 616-87-5 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E+00	3.850E+02	0	M051	1 0 0 0 2	
2.974E+00	5.180E+02	15	M051	1 0 0 0 2	
3.490E+00	6.080E+02	25	M051	1 0 0 0 2	
4.788E+00	8.340E+02	50	M051	1 0 0 0 2	

1582. $C_8H_{14}O_4$
Propyl α-acetoxypropionate
Hydracrylic acid, propyl ester, acetate
RN: 20473-73-8 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.683E-02	9.900E+00	25	R006	2 2 0 1 1	

1583. $C_8H_{14}O_4$
Ethylene glycol dipropionate
1,2-Ethanediol, dipropanoate
1,2-bis(Propionyloxy)ethane
RN: 123-80-8 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.480E-02	1.651E+01	25	F064	1 0 0 0 2	
9.170E-03	1.597E+00	ns	F014	0 0 0 0 2	

1584. $C_8H_{14}O_5$
Propanoic acid, 2-[(propoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 190.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	5.173E+00	25	R007	0 0 0 0 0	

1585. $C_8H_{15}ClN_5O$
Hydroxyatrazine
4-(Ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2(1H)-one
2-Hydroxy atrazine
RN: 2163-68-0 **MP** (°C)**:**
MW: 232.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.585E-02	2	B193	1 2 0 0 1	

1586. $C_8H_{15}NO$
Pelletierine
Pelletierin
RN: 2858-66-4 **MP** (°C)**:** <25
MW: 141.21 **BP** (°C)**:** 195

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-01	5.000E+01	20	F300	1 0 0 0 0	
3.372E-01	4.762E+01	25	D004	0 0 0 0 0	

1587. $C_8H_{15}NO$
Propylallylacetamide
2-Propyl-4-pentenamide
PAD
RN: 90204-40-3 **MP** (°C)**:**
MW: 141.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-02	9.500E+00	37	H347	0 0 0 0 0	

1588. $C_8H_{15}NO_2S$
4-Thiazolidinecarboxylic acid, 2-butyl-
RN: 90205-28-0 **MP** (°C)**:**
MW: 189.28 **BP** (°C)**:** 355.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.079E+01	21	B414	1 0 0 1 1	partial decomposition

1589. $C_8H_{15}NO_2S$
4-Thiazolidinecarboxylic acid, 2-(2-methylpropyl)-
4-Thiazolidine-4-carboxylic acid, 2-(2-isobutyl)-
RN: 215669-71-9 **MP** (°C)**:**
MW: 189.28 **BP** (°C)**:** 347.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	9.275E+00	21	B414	1 0 0 1 1	partial decomposition

1590. $C_8H_{15}N_3O_2$
Isocarbamid
N-(2-Methylpropyl)-2-oxo-1-imidazolidinecarboxamide
RN: 30979-48-7 **MP** (°C)**:** 95.5
MW: 185.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.018E-03	1.300E+00	20	M161	1 0 0 0 1	

1591. $C_8H_{15}N_3O_7$

Streptozotocin
Streptozocin
D-2-Deoxy-2-(3-methyl-3-nitrosoureido)glucopyranose
RN: 18883-66-4 **MP** (°C)**:** 115
MW: 265.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-02	5.066E+00	25	I307	0 0 0 0 0	

1592. $C_8H_{15}N_5O$

Simetone
2-Methoxy-4,6-bis(ethylamino)-*s*-triazine
s-Triazole, 2,4-bis(ethylamine)-6-methoxy-
RN: 673-04-1 **MP** (°C)**:** 118-120
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.622E-02	3.200E+00	21	B185	0 0 0 0 0	
1.622E-02	3.200E+00	21	B192	0 0 0 0 2	
1.622E-02	3.200E+00	21	G099	2 0 0 1 0	
3.550E-02	7.002E+00	50	G001	1 0 1 1 2	
1.622E-02	3.200E+00	ns	C101	0 0 0 0 1	

1593. $C_8H_{15}N_5O$

2-Methoxy-4-methylamino-6-isopropylamino-*s*-triazine
Noratone
RN: 3035-45-8 **MP** (°C)**:**
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.774E-02	3.500E+00	20	J033	0 0 0 0 0	
1.774E-02	3.500E+00	21	B192	0 0 0 0 2	

1594. $C_8H_{15}N_5S$

Desmetryne
N-Methyl-*N*′-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
Semeron
Methylamino-4-methylthio-6-isopropylamino-1,3,5-triazine
Topusyn
Methylthio-4-isopropylamino-6-methylamino-*s*-triazine
RN: 1014-69-3 **MP** (°C)**:**
MW: 213.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-03	6.000E-01	20	F311	1 2 2 2 1	
2.719E-03	5.800E-01	20	M161	1 0 0 0 2	
2.811E-03	5.996E-01	ns	B100	0 0 0 0 0	

(*continued*)

1594. $C_8H_{15}N_5S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	5.800E-01	ns	J033	0 0 0 0 0	
2.719E-03	5.800E-01	ns	M061	0 0 0 0 2	

1595. $C_8H_{15}N_5S$

Simetryne
N,N′-Diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
G-32911
bis(Ethylamino)-6-(methylthio)-*s*-triazine
Methylthio-4,6-bis(ethylamino)-*s*-triazine
Cymetrin

RN: 1014-70-6 **MP** (°C)**:** 82
MW: 213.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	1.003E+00	50	G001	1 0 1 1 1	
2.110E-03	4.500E-01	ns	C101	0 0 0 0 1	
2.110E-03	4.500E-01	ns	J033	0 0 0 0 0	
2.110E-03	4.500E-01	rt	M161	0 0 0 0 2	

1596. $C_8H_{15}N_7O_2S_3$

Famotidine
Amfamox
N′-(Aminosulfonyl)-3-(((2-(((diaminomethylene)amino)-4-thiazolyl)methyl)thio)propanimidamide
Pepcid
Pepcidine
Pepcid PM

RN: 76824-35-6 **MP** (°C)**:**
MW: 337.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.260E-06	1.100E-03	25	A408	2 0 1 2 0	
3.311E-03	1.117E+00	ns	R427	0 0 0 0 0	

1597. C_8H_{16}

Cyclooctane

RN: 292-64-8 **MP** (°C)**:** 10
MW: 112.22 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-03	1.817E-01	20	M337	2 1 2 2 2	*sic*
7.040E-05	7.900E-03	25	M001	2 1 2 2 1	
7.040E-05	7.900E-03	ns	H123	0 0 0 0 0	

1598. C_8H_{16}
Caprylene
1-Octene
RN: 111-66-0 **MP** (°C)**:** –102
MW: 112.22 **BP** (°C)**:** 121.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-05	3.600E-03	23	C332	0 0 0 0 0	
2.406E-05	2.700E-03	25	M001	2 1 2 2 1	
3.650E-05	4.096E-03	25	M342	1 0 1 1 2	

1599. C_8H_{16}
1,4-Dimethylcyclohexane
p-Dimethylcyclohexane
RN: 589-90-2 **MP** (°C)**:** –87
MW: 112.22 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	K119	1 0 0 0 2	

1600. C_8H_{16}
cis-1,2-Dimethylcyclohexane
1-*cis*-2-Dimethylcyclohexane
RN: 2207-01-4 **MP** (°C)**:** –50
MW: 112.22 **BP** (°C)**:** 129

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.773E-05	7.600E-03	20	M337	2 1 2 2 1	
5.347E-05	6.000E-03	25	M001	2 1 2 2 1	

1601. C_8H_{16}
n-Propylcyclopentane
1-Propylcyclopentane
RN: 2040-96-2 **MP** (°C)**:** –117
MW: 112.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.818E-05	2.040E-03	25	K119	1 0 0 0 2	
1.818E-05	2.040E-03	25	P051	2 1 1 2 2	
1.818E-05	2.040E-03	25.00	P007	2 1 2 2 2	

1602. C_8H_{16}
trans-1,2-Dimethylcyclohexane
1,2-*trans*-Dimethylcyclohexane
RN: 6876-23-9 **MP** (°C)**:** –89
MW: 112.22 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-05	5.200E-03	20	M337	2 1 2 2 1	
4.444E-05	4.987E-03	30.2	M447	0 0 0 0 0	
1.061E-04	1.191E-02	70.3	M447	0 0 0 0 0	
2.611E-04	2.930E-02	100.7	M447	0 0 0 0 0	
6.000E-04	6.733E-02	131.0	M447	0 0 0 0 0	
1.239E-03	1.390E-01	151.0	M447	0 0 0 0 0	
1.977E-03	2.219E-01	170.1	M447	0 0 0 0 0	

1603. C_8H_{16}
trans-1,4-Dimethylcyclohexane
1,4-Transdimethylcyclohexane
RN: 2207-04-7 **MP** (°C)**:** –37
MW: 112.22 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	P051	2 1 1 2 2	
3.422E-05	3.840E-03	25.00	P007	2 1 2 2 2	

1604. C_8H_{16}
1,2-Dimethylcyclohexane (*cis* + *trans*)
Cyclohexane, 1,2-dimethyl- (*cis*/*trans*)
1,2-Dimethylcyclohexane
RN: 583-57-3 **MP** (°C)**:**
MW: 112.22 **BP** (°C)**:** 124 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.056E-05	6.795E-03	30.0	M447	0 0 0 0 0	
1.200E-04	1.347E-02	70.0	M447	0 0 0 0 0	
2.422E-04	2.718E-02	100.2	M447	0 0 0 0 0	
5.483E-04	6.153E-02	130.5	M447	0 0 0 0 0	
1.089E-03	1.222E-01	150.5	M447	0 0 0 0 0	
2.422E-03	2.717E-01	170.5	M447	0 0 0 0 0	

1605. C_8H_{16}
1,1,3-Trimethylcyclopentane
Cyclopentane, 1,1,3-trimethyl-
RN: 4516-69-2 **MP** (°C)**:** –142.4
MW: 112.22 **BP** (°C)**:** 104.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.324E-05	3.730E-03	25	K119	1 0 0 0 2	
3.324E-05	3.730E-03	25	P051	2 1 1 2 2	
3.324E-05	3.730E-03	25.00	P007	2 1 2 2 2	

1606. C_8H_{16}
Ethyl cyclohexane
Cyclohexane, ethyl-
RN: 1678-91-7 **MP** (°C)**:**
MW: 112.22 **BP** (°C)**:** 131.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.614E-05	6.300E-03	20	M337	2 1 2 2 1	
3.883E-05	4.358E-03	30.3	M447	0 0 0 0 0	
7.833E-05	8.790E-03	70.4	M447	0 0 0 0 0	
2.511E-04	2.818E-02	100.5	M447	0 0 0 0 0	
6.055E-04	6.795E-02	131.0	M447	0 0 0 0 0	
9.871E-04	1.108E-01	151.2	M447	0 0 0 0 0	
1.633E-03	1.833E-01	170.8	M447	0 0 0 0 0	

1607. $C_8H_{16}Br_2$
1,8-Dibromooctane
Octamethylene dibromide
RN: 4549-32-0 **MP** (°C)**:** 15–16
MW: 272.03 **BP** (°C)**:** 270–272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.389E-06	2.010E-03	1.0	S464	0 0 0 0 0	
7.278E-06	1.980E-03	1.0	S464	0 0 0 0 0	
7.462E-06	2.030E-03	4.9	S464	0 0 0 0 0	
7.646E-06	2.080E-03	4.9	S464	0 0 0 0 0	
8.565E-06	2.330E-03	10.0	S464	0 0 0 0 0	
8.896E-06	2.420E-03	14.9	S464	0 0 0 0 0	
8.528E-06	2.320E-03	14.9	S464	0 0 0 0 0	
9.374E-06	2.550E-03	19.9	S464	0 0 0 0 0	
1.062E-05	2.890E-03	25	S464	0 0 0 0 0	
1.066E-05	2.900E-03	25.0	S464	0 0 0 0 0	
1.044E-05	2.840E-03	25.0	S464	0 0 0 0 0	
1.209E-05	3.290E-03	30.0	S464	0 0 0 0 0	
1.239E-05	3.370E-03	30.0	S464	0 0 0 0 0	
1.213E-05	3.300E-03	30.1	S464	0 0 0 0 0	

(*continued*)

1607. $C_8H_{16}Br_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E-05	3.430E-03	34.9	S464	0 0 0 0 0	
1.309E-05	3.560E-03	35.0	S464	0 0 0 0 0	
1.430E-05	3.890E-03	40.1	S464	0 0 0 0 0	
1.386E-05	3.770E-03	40.1	S464	0 0 0 0 0	

1608. $C_8H_{16}Cl_2$

1,8-Dichlorooctane

RN: 2162-99-4 **MP** (°C)**:** –8
MW: 183.12 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-05	4.470E-03	3.6	S464	0 0 0 0 0	
3.047E-05	5.580E-03	5.1	S464	0 0 0 0 0	
3.014E-05	5.520E-03	5.1	S464	0 0 0 0 0	
3.069E-05	5.620E-03	9.9	S464	0 0 0 0 0	
3.233E-05	5.920E-03	15.1	S464	0 0 0 0 0	
3.211E-05	5.880E-03	25.1	S464	0 0 0 0 0	
3.255E-05	5.960E-03	25.1	S464	0 0 0 0 0	
3.222E-05	5.900E-03	25.1	S464	0 0 0 0 0	
3.517E-05	6.440E-03	30.3	S464	0 0 0 0 0	
3.375E-05	6.180E-03	30.3	S464	0 0 0 0 0	
3.823E-05	7.000E-03	35.2	S464	0 0 0 0 0	
3.828E-05	7.010E-03	35.3	S464	0 0 0 0 0	
3.970E-05	7.270E-03	40.1	S464	0 0 0 0 0	

1609. $C_8H_{16}N_2O_2$

N,N,N′,N′-Tetramethylsuccinamide
N,N,N′,N′-Tetramethylbutanediamide

RN: 7334-51-2 **MP** (°C)**:**
MW: 172.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.188E+00	5.490E+02	30	K004	1 0 0 0 2	

1610. $C_8H_{16}N_2O_4S_2$

DL-Homocystine
DL-*meso*-Homocystine
Oxidized DL-homocysteine

RN: 870-93-9 **MP** (°C)**:** 264
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.451E-04	2.000E-01	25	D041	1 0 0 0 0	

1611. $C_8H_{16}N_6$
Pentamethylmelamine
1-(Methylamino)-3,5-bis(dimethylamino)-*s*-triazine
RN: 16268-62-5 **MP** (°C)**:** 107.0
MW: 196.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.679E-04	3.295E-02	25	B386	0 0 0 0 0	
1.010E-02	1.982E+00	25	B386	0 0 0 0 0	
1.101E-02	2.160E+00	25	C051	1 2 1 1 2	pH 7

1612. $C_8H_{16}N_6O$
*N*2-Hydroxy-*N*2,*N*4,*N*4,*N*6,*N*6-pentamethylmelamine
1-(Hydroxylamino)-3,5-bis(dimethylamino)-*s*-triazine
RN: 64124-14-7 **MP** (°C)**:** 110.0
MW: 212.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.412E-03	9.365E-01	25	B386	0 0 0 0 0	
4.259E-03	9.040E-01	25	C051	1 2 1 1 2	pH 7

1613. $C_8H_{16}O$
Cyclooctanol
RN: 696-71-9 **MP** (°C)**:** 15
MW: 128.22 **BP** (°C)**:** 106–108 at 22 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.129E-02	6.576E+00	ns	S460	0 0 0 0 0	

1614. $C_8H_{16}O$
1-Octen-3-ol
3-Octenol
Flowtron mosquito attractant
Matsuka alcohol
Vinyl hexanol
RN: 3391-86-4 **MP** (°C)**:**
MW: 128.22 **BP** (°C)**:** 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.557E-02	1.996E+00	25	D425	0 0 0 0 0	

1615. $C_8H_{16}O$
Hexyl methyl ketone
2-Octanone
Octan-2-one
RN: 111-13-7 **MP** (°C)**:** –16.0
MW: 128.22 **BP** (°C)**:** 172.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.276E-02	4.200E+00	0	C423	0 0 0 0 0	
2.574E-02	3.300E+00	4	C423	0 0 0 0 0	
1.716E-02	2.200E+00	10	C423	0 0 0 0 0	
7.013E-03	8.992E-01	20	D052	1 1 0 0 0	
1.014E-02	1.300E+00	25	C435	0 0 0 0 0	

1616. $C_8H_{16}O$
Caprylic aldehyde
Octaldehyde
n-Octanal
RN: 124-13-0 **MP** (°C)**:**
MW: 128.22 **BP** (°C)**:** 163.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.368E-03	5.600E-01	25	A049	1 0 0 0 1	
1.887E-03	2.420E-01	25	L450	0 0 0 0 0	

1617. $C_8H_{16}O_2$
Ethyl hexanoate
Ethyl butyl acetate
Ethyl caproate
Ethyl *n*-hexanoate
Ethyl caproate (Nat. C-6 ethyl ester)
RN: 123-66-0 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.500E-01	0	C423	0 0 0 0 0	
3.606E-03	5.200E-01	4	C423	0 0 0 0 0	
3.952E-03	5.700E-01	10	C423	0 0 0 0 0	
4.507E-03	6.500E-01	25	C435	0 0 0 0 0	
4.467E-03	6.442E-01	ns	S460	0 0 0 0 0	

1618. $C_8H_{16}O_2$
Valproic acid
Vistora
Valporal
Convulex
Depakote
Dalpro
RN: 99-66-1 **MP** (°C)**:** 120–130
MW: 144.22 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.014E-03	1.300E+00	ns	K444	0 0 0 0 0	
1.380E-02	1.991E+00	ns	S460	0 0 0 0 0	

1619. $C_8H_{16}O_2$
2-Ethylhexoic acid
2-Ethyl-1-hexanoic acid
3-Heptanecarboxylic acid
Butylethylacetic acid
RN: 149-57-5 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-02	1.498E+00	25	O011	1 0 1 1 1	

1620. $C_8H_{16}O_2$
3-Hydroxy-2,2,5,5-tetramethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-2,2,5,5-tetramethyl-
RN: 29839-74-5 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.304E-01	9.091E+01	rt	B066	0 2 0 0 1	

1621. $C_8H_{16}O_2$
n-Butyl *n*-butyrate
Butyl butyrate
RN: 109-21-7 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-03	4.998E-01	20	D052	1 1 0 0 0	

1622. $C_8H_{16}O_2$
Pentyl propionate
Propanoic acid pentyl ester
Amyl *n*-propanoate
n-Pentyl propionate
RN: 624-54-4 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	7.067E-01	20	S006	1 0 0 0 1	

1623. $C_8H_{16}O_2$
3-Hydroxy-2,2-diethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1624. $C_8H_{16}O_2$
sec-Hexyl acetate
Methyl amyl acetate
RN: 108-84-9 **MP** (°C)**:** –64
MW: 144.22 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.543E-03	7.994E-01	20	D052	1 1 0 0 0	

1625. $C_8H_{16}O_2$
Isobutyl isobutyrate
Isobutyl 2-methylpropanoate
2-Methylpropyl 2-methylpropanoate
IBIB
RN: 97-85-8 **MP** (°C)**:** –81
MW: 144.22 **BP** (°C)**:** 147

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-03	5.700E-01	25	A049	1 0 0 0 1	

1626. $C_8H_{16}O_2$
3-Hydroxy-2-ethyl-5,5-dimethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5,5-dimethyl-
RN: 29839-59-6 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.302E-01	4.762E+01	rt	B066	0 2 0 0 0	

1627. $C_8H_{16}O_2$
3-Hydroxy-5-ethyl-2,5-dimethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-2,5-dimethyl-
RN: 29839-60-9 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E+00	5.000E+02	rt	B066	0 2 0 0 2	

1628. $C_8H_{16}O_2$
3-Hydroxy-5-methyl-5-propyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5-methy-5-propyl-
RN: 29839-52-9 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1629. $C_8H_{16}O_2$
Hexyl acetate
2-Ethyl butyl acetate
RN: 142-92-7 **MP** (°C)**:** –80
MW: 144.22 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.158E-03	5.996E-01	20	D052	1 1 0 0 0	
3.540E-03	5.105E-01	25	M124	2 1 2 2 2	

1630. $C_8H_{16}O_2$
Caprylic acid
Caprylsaure
RN: 124-07-2 **MP** (°C)**:** 16.7
MW: 144.22 **BP** (°C)**:** 239.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-03	4.400E-01	0	B136	1 0 2 1 1	
4.993E-03	7.200E-01	15	F300	1 0 0 0 1	
4.715E-03	6.800E-01	20	B136	1 0 2 1 1	
4.712E-03	6.795E-01	20	D041	1 0 0 0 1	
4.712E-03	6.795E-01	20.0	R001	1 1 1 1 1	
5.478E-03	7.900E-01	30	B136	1 0 2 1 1	
5.471E-03	7.890E-01	30	E005	2 1 1 2 2	
5.474E-03	7.894E-01	30.0	R001	1 1 1 1 1	
5.845E-03	8.430E-01	40	E005	2 1 1 2 2	
6.587E-03	9.500E-01	45	B136	1 0 2 1 1	
6.581E-03	9.491E-01	45.0	R001	1 1 1 1 1	
6.539E-03	9.430E-01	50	E005	2 1 1 2 2	
7.835E-03	1.130E+00	60	B136	1 0 2 1 2	
7.426E-03	1.071E+00	60	E005	2 1 1 2 2	
7.827E-03	1.129E+00	60.0	R001	1 1 1 1 2	
1.803E-02	2.600E+00	100	F300	1 0 0 0 1	
3.050E-03	4.398E-01	.0	R001	1 1 1 1 1	

1631. $C_8H_{16}O_3$
n-Butyl β-methoxypropionate
Propanoic acid, 3-methoxy-, butyl ester
RN: 4195-88-4 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.117E-02	9.800E+00	25	R034	0 0 0 0 1	

1632. $C_8H_{16}O_3$
Amyl lactate
n-Pentyl lactate
RN: 6382-06-5 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-02	1.000E+01	25	R006	2 2 0 1 2	

1633. $C_8H_{16}O_3$
Methyl β-*n*-butoxypropionate
Butanoic acid, 3-methoxy-3-oxopropyl ester
RN: 40326-33-8 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.076E-02	8.133E+00	25	R034	0 0 0 0 1	

1634. $C_8H_{16}O_3$
n-Propyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, propyl ester
RN: 14144-34-4 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.466E-02	1.517E+01	25	D002	1 2 1 1 2	

1635. $C_8H_{16}O_3$
Butylcellosolve acetate
Ethylene glycol monobutyl ether acetate
Ektasolve EB acetate
n-Butyl cellosolve acetate
Ethylene glycol mono-*n*-butyl ether acetate
RN: 112-07-2 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.567E-02	8.920E+00	20	D052	1 1 0 0 0	

1636. $C_8H_{16}O_3$
2,2,5,5-Tetramethyltetrahydrofuran-3,4-diol
3,4-Furandiol, tetrahydro-2,2,5,5-tetramethyl-
RN: 29839-67-6 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.674E-01	9.091E+01	rt	B066	0 2 0 0 1	

1637. $C_8H_{16}O_3S$
1,2-Oxathiolane, 5-pentyl-, 2,2-dioxide
1-Octanesulfonic acid, 3-hydroxy-, γ-sultone
RN: 5633-87-4 **MP** (°C)**:**
MW: 192.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.499E-01	20	B058	1 2 0 0 1	
7.938E-02	1.526E+01	100	B058	1 2 0 0 2	

1638. $C_8H_{16}O_4$
Metaldehyde
Acetaldehyde homopolymer
Acetaldehyde tetramer
RN: 9002-91-9 **MP** (°C)**:** 112
MW: 176.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	2.000E-01	17	M161	1 0 0 0 2	

1639. $C_8H_{17}Cl$
1-Chlorooctane
1-Octylchloride
n-Octyl chloride
Octyl chloride
RN: 111-85-3 **MP** (°C)**:** –61
MW: 148.68 **BP** (°C)**:** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E+01	3.375E+03	5.0	S454	0 0 0 0 0	
2.210E+01	3.286E+03	10.0	S454	0 0 0 0 0	
2.260E+01	3.360E+03	9.9	S454	0 0 0 0 0	
2.350E+01	3.494E+03	9.9	S454	0 0 0 0 0	
2.370E+01	3.524E+03	9.9	S454	0 0 0 0 0	
2.540E+01	3.776E+03	19.1	S454	0 0 0 0 0	
2.470E+01	3.672E+03	25.0	S454	0 0 0 0 0	
2.620E+01	3.895E+03	25.1	S454	0 0 0 0 0	
2.580E+01	3.836E+03	25.2	S454	0 0 0 0 0	
2.710E+01	4.029E+03	30.0	S454	0 0 0 0 0	
2.700E+01	4.014E+03	34.8	S454	0 0 0 0 0	
2.800E+01	4.163E+03	35.1	S454	0 0 0 0 0	
2.690E+01	3.999E+03	35.1	S454	0 0 0 0 0	
2.750E+01	4.089E+03	40.0	S454	0 0 0 0 0	

1640. $C_8H_{17}N$
D-Coniine
α-Propylpiperidine
D-Coniin
Coniine
RN: 458-88-8 **MP** (°C)**:** –2
MW: 127.23 **BP** (°C)**:** 166–167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	1.800E+01	19.5	F300	1 0 0 0 1	
7.782E-02	9.901E+00	25	D004	0 0 0 0 0	

1641. $C_8H_{17}NO$
Ethylbutylacetamide
2-Ethylhexanamide
EBD
RN: 4164-92-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.072E-02	4.400E+00	37	H347	0 0 0 0 0	

1642. $C_8H_{17}NO$
Ethylisobutylacetamide
2-Ethyl-4-methylpentanamide
EID
RN: 130482-28-9 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1643. $C_8H_{17}NO$
Caprylylamide
Caprylsaeure-amid
RN: 629-01-6 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.288E-02	4.710E+00	100	F300	1 0 0 0 2	

1644. $C_8H_{17}NO$
Propylisopropylacetamide
2-Isopropyl-2-propylacetamide
2-Isopropylvaleramide
PID
RN: 6098-19-7 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.444E-02	3.500E+00	37	H347	0 0 0 0 0	

1645. $C_8H_{17}NO$
2-Isopropyl-3-methyl-butyramide
3-Methyl-2-(1-methylethyl)butanamide
Diisopropylacetamide
RN: 5440-65-3 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1646. $C_8H_{17}NO$
Dimethylbutylacetamide
2,2-Dimethylhexanamide
DBD
RN: 20923-67-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.374E-02	3.400E+00	ns	H348	0 0 0 0 0	

1647. $C_8H_{17}NO$
Valnoctamide
VCD
Valmethamide
2-Ethyl-3-methyl-pentanamide
RN: 4171-13-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.074E-02	8.700E+00	ns	H348	0 0 0 0 0	

1648. $C_8H_{17}NO$
Methylpentylacetamide
2-Methyl-heptanamide
MPD
RN: 4164-91-4 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.957E-02	7.100E+00	37	H347	0 0 0 0 0	

1649. $C_8H_{17}NO_2$
n-Heptyl carbamate
Heptyl carbamate
RN: 4248-20-8 **MP** (°C)**:** 66
MW: 159.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	3.822E-01	37	H006	1 2 2 1 1	

1650. $C_8H_{17}NO_3$
N-Isoamylurethane
RN: **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.329E-02	4.082E+00	20	O021	1 0 0 0 0	

1651. C_8H_{18}
2,3,4-Trimethylpentane
2,3,4-Trojmetylopentan
RN: 565-75-3 **MP** (°C)**:** –110
MW: 114.23 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-05	2.340E-03	0	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	K119	1 0 0 0 2	
2.013E-05	2.300E-03	25	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	P051	2 1 1 2 2	
1.191E-05	1.360E-03	25.00	P007	2 1 2 2 2	

1652. C_8H_{18}
3-Methylheptane
3-Metyloheptan
RN: 589-81-1 **MP** (°C)**:** –121
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.539E-05	2.900E-03	23	C332	0 0 0 0 0	
6.933E-06	7.920E-04	25	K119	1 0 0 0 2	
6.933E-06	7.920E-04	25	P051	2 1 1 2 2	
6.933E-06	7.920E-04	25.00	P007	2 1 2 2 2	

1653. C_8H_{18}
Isooctane
2:2:4-Trimethylpentane
RN: 540-84-1 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-05	2.460E-03	0	P003	2 2 2 2 2	
1.226E-05	1.400E-03	20	M337	2 1 2 2 1	
9.980E-06	1.140E-03	25	K119	1 0 0 0 2	
2.136E-05	2.440E-03	25	M001	2 1 2 2 2	
2.136E-05	2.440E-03	25	M002	2 1 2 2 2	
2.136E-05	2.440E-03	25	M130	1 0 0 0 2	
1.795E-05	2.050E-03	25	P003	2 2 2 2 2	
9.980E-06	1.140E-03	25	P051	2 1 1 2 2	
9.980E-06	1.140E-03	25.00	P007	2 1 2 2 2	
7.879E-06	9.000E-04	ns	B170	0 0 0 0 2	
7.500E-05	8.567E-03	ns	J300	0 0 0 0 0	

1654. C_8H_{18}
3,4-Dimethylhexane
RN: 583-48-2 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.998E-06	7.994E-04	ns	S460	0 0 0 0 0	

1655. C_8H_{18}
3-Ethylhexane
Ethyl hexane
RN: 619-99-8 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.076E-06	3.514E-04	ns	S460	0 0 0 0 0	

1656. C_8H_{18}
2,4-Dimethylhexane
RN: 589-43-5 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-05	1.294E-03	ns	S460	0 0 0 0 0	

1657. C_8H_{18}
2,3-Dimethylhexane
2:3-Dimethylhexane
RN: 590-73-8 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.751E-06	2.000E-04	ns	B170	0 0 0 0 2	

1658. C_8H_{18}
2-Methylheptane
RN: 592-27-8 **MP** (°C)**:** –109
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-05	3.800E-03	23	C332	0 0 0 0 0	

1659. $C_8H_{18}NO_4PS_2$
Vamidothion
O,O-Dimethyl *S*-2-(1-*N*-methylcarbamoylethylmercapto)ethyl thiophosphate
RN: 2275-23-2 **MP** (°C)**:** 35.5
MW: 287.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E+01	4.000E+03	20	M161	1 0 0 0 0	
1.392E+01	4.000E+03	ns	M061	0 0 0 0 2	

1660. $C_8H_{18}N_2O$
Di-*n*-butylnitrosamine
N-Nitroso-di-*n*-butylamine
Dibutylnitrosamine
RN: 924-16-3 **MP** (°C)**:**
MW: 158.25 **BP** (°C)**:** 234

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.266E+00	24	D083	2 0 0 0 0	
7.574E-03	1.199E+00	rt	I307	0 0 0 0 0	

1661. $C_8H_{18}O$
2-Octanol
sec-Caprylic alcohol
sec-Octyl alcohol
Methyl hexyl carbinol
RN: 123-96-6 **MP** (°C)**:** –38.6
MW: 130.23 **BP** (°C)**:** 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-02	1.508E+00	15	M073	1 0 2 2 2	
8.131E-03	1.059E+00	20	A015	1 2 1 1 2	
8.600E-03	1.120E+00	20	H330	0 0 0 0 0	
3.059E-02	3.984E+00	25	C093	2 1 1 1 0	
9.829E-03	1.280E+00	25	M073	1 0 2 2 2	
7.892E-03	1.028E+00	ns	J300	0 0 0 0 0	

1662. $C_8H_{18}O$
bis(2-Methyl propyl) ether
iso-Butyl ether
Di-isobutyl ether
RN: 628-55-7 **MP** (°C)**:**
MW: 130.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.059E+00	1.379E+02	25	M375	2 2 2 1 1	
1.227E-02	1.597E+00	51	M375	2 2 2 1 1	
1.002E+00	1.304E+02	60	M375	2 2 2 1 1	

1663. $C_8H_{18}O$
DL-2-Octanol
DL-Octanol-(2)
RN: 4128-31-8 **MP** (°C)**:** –31.6
MW: 130.23 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-02	1.500E+00	15	F300	1 0 0 0 1	
9.214E-03	1.200E+00	25	F300	1 0 0 0 1	

1664. $C_8H_{18}O$

2-Ethyl-1-hexanol
Octyl alcohol
Octyl-(2-ethyl hexyl) alcohol
2-Ethyl hexanol
2-Ethylhexanol
2-Ethylhexan-1-ol

RN: 104-76-7 **MP** (°C)**:** –76
MW: 130.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.318E+00	10.2	S307	1 1 0 2 2	
9.586E-03	1.248E+00	19.8	S307	1 1 0 2 2	
4.604E-03	5.996E-01	20	D052	1 1 0 0 0	
6.760E-03	8.804E-01	20	H330	0 0 0 0 0	
9.982E-04	1.300E-01	25	K072	1 0 1 1 1	
7.441E-03	9.691E-01	29.6	S307	1 1 0 2 1	
8.437E-03	1.099E+00	40.1	S307	1 1 0 2 2	
5.678E-03	7.395E-01	50.2	S307	1 1 0 2 1	
6.598E-03	8.593E-01	60.3	S307	1 1 0 2 1	
7.594E-03	9.890E-01	70.1	S307	1 1 0 2 1	
8.284E-03	1.079E+00	80.1	S307	1 1 0 2 2	
8.973E-03	1.169E+00	90.3	S307	1 1 0 2 2	

1665. $C_8H_{18}O$

1-Octanol
Caprylic alcohol
n-Octyl alcohol
n-Octanol

RN: 111-87-5 **MP** (°C)**:** –16
MW: 130.23 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-03	4.198E-01	20	A015	1 2 1 1 2	
3.680E-03	4.793E-01	20	H330	0 0 0 0 0	
3.761E-03	4.898E-01	20.5	S307	1 1 0 2 1	
3.236E-03	4.214E-01	20.96	B178	1 1 0 1 2	EFG
3.162E-03	4.118E-01	23.58	B178	1 1 0 1 2	EFG
2.700E-03	3.516E-01	24	H345	0 0 0 0 0	
4.497E-03	5.857E-01	25	B038	1 2 1 1 2	
3.820E-02	4.975E+00	25	C093	2 1 1 1 0	*sic*
1.000E+00	1.302E+02	25	F044	1 0 0 0 0	EFG
1.060E-03	1.380E-01	25	J035	0 0 0 0 0	
3.830E-03	4.988E-01	25	J302	2 1 2 2 2	
3.800E-03	4.949E-01	25	K025	2 2 1 1 2	
4.530E-03	5.900E-01	25	K072	1 0 1 1 1	
3.970E-03	5.170E-01	25	L322	1 1 2 2 1	
4.530E-03	5.900E-01	25	M087	1 1 2 1 1	
4.110E-03	5.353E-01	25	S359	2 1 2 2 2	

(*continued*)

1665. $C_8H_{18}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.671E-03	9.990E-01	30	R067	0 0 0 0 0	
4.911E-03	6.396E-01	30.6	S307	1 1 0 2 1	
3.236E-03	4.214E-01	34.53	B178	1 1 0 1 2	EFG
1.075E-03	1.400E-01	40	J035	0 0 0 0 0	
4.988E-03	6.496E-01	40.1	S307	1 1 0 2 1	
8.054E-03	1.049E+00	50.0	S307	1 1 0 2 2	
3.548E-03	4.621E-01	60	B178	1 1 0 1 2	EFG
6.751E-03	8.792E-01	60.3	S307	1 1 0 2 1	
3.548E-03	4.621E-01	69.31	B178	1 1 0 1 2	EFG
5.908E-03	7.694E-01	70.3	S307	1 1 0 2 1	
6.675E-03	8.692E-01	80.1	S307	1 1 0 2 1	
6.598E-03	8.593E-01	90.3	S307	1 1 0 2 1	
4.514E-03	5.879E-01	ns	L003	0 0 2 1 2	

1666. $C_8H_{18}O$
n-Butyl ether
Butyl ether
Dibutyl ether
RN: 142-96-1 **MP** (°C)**:** –98
MW: 130.23 **BP** (°C)**:** 142.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E-02	1.847E+00	24.80	O005	2 0 2 2 2	
2.700E-03	3.516E-01	25	K012	1 0 0 0 1	
6.138E-03	7.994E-01	25.50	O005	2 0 2 2 0	
1.720E-02	2.240E+00	37	E028	1 0 1 1 2	

1667. $C_8H_{18}O_2$
Ethohexadiol
2-Ethyl-1,3-hexanediol
RN: 94-96-2 **MP** (°C)**:** –40
MW: 146.23 **BP** (°C)**:** 244.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.103E-02	6.000E+00	20	M161	1 0 0 0 0	
2.756E-01	4.031E+01	25	C093	2 1 1 1 1	
2.756E-01	4.031E+01	ns	M061	0 0 0 0 1	

1668. $C_8H_{18}O_4S_2$
Sulfonethylmethane
Trional
RN: 76-20-0 **MP** (°C)**:** 75
MW: 242.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-02	4.975E+00	16	A072	1 0 1 0 1	
2.063E-02	5.000E+00	16	F300	1 0 0 0 0	
2.042E-02	4.948E+00	ns	R427	0 0 0 0 0	

1669. $C_8H_{19}N$
Octylamine
1-Aminooctane
1-Octanamine
Monoctylamine
n-Octylamine
RN: 111-86-4 **MP** (°C)**:** –5
MW: 129.25 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.547E-03	2.000E-01	25	K072	1 0 1 1 1	
1.547E-03	2.000E-01	25	M087	1 1 2 1 1	

1670. $C_8H_{19}N$
n-Dibutylamine
Di-*n*-butylamine
N,N-Dibutylamine
N-Butyl-1-butanamine
RN: 111-92-2 **MP** (°C)**:** –62
MW: 129.25 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.231E+00	25	K012	1 0 0 0 1	

1671. $C_8H_{19}O_2PS_2$
Ethoprop
Ethoprophos
O-Ethyl-*S,S*-dipropylphosphorodithioate
Holdem
Rovokil
Ethyl *S,S*-dipropyl phosphorodithioate
RN: 13194-48-4 **MP** (°C)**:**
MW: 242.34 **BP** (°C)**:** 88.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.095E-03	7.500E-01	ns	M161	0 0 0 0 2	
3.097E-03	7.506E-01	ns	S460	0 0 0 0 0	

1672. $C_8H_{19}O_2PS_3$
Disulfoton
Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester
Solvirex
Disyston
Thiodemeton
Ethylthiometon
RN: 298-04-4 **MP** (°C)**:** 108
MW: 274.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.940E-05	1.630E-02	19.50	B169	2 1 1 1 2	
9.111E-05	2.500E-02	20	M061	1 0 0 0 1	
5.888E-05	1.616E-02	ns	S460	0 0 0 0 0	
9.111E-05	2.500E-02	rt	M161	0 0 0 0 1	

1673. $C_8H_{19}O_3P$
Dibutyl hydrogen phosphonate
Di-*n*-butyl phosphite
Dibutoxyphosphine oxide
RN: 1809-19-4 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.759E-02	7.300E+00	25	B070	1 2 0 1 1	

1674. $C_8H_{19}O_3PS_2$
Demetonthione
Thiophosphorsaeure-*O,O*-diaethyl-*O*-[2-(aethylthio)-aethyl]-ester
O,O-Diethyl-*O*-(2-(ethylthio)-ethyl)ester thiophosphoric acid
O,O-Diethyl 2-ethylmercaptoethyl thiophosphate
Systox
Thiolo-demeton
RN: 298-03-3 **MP** (°C)**:**
MW: 258.34 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-04	6.000E-02	20	M061	1 0 0 0 1	
7.742E-03	2.000E+00	rt	M161	0 0 0 0 0	form II
2.323E-04	6.000E-02	rt	M161	0 0 0 0 1	form I
1.277E-02	3.300E+00	rt	M161	0 0 0 0 1	

1675. $C_8H_{19}O_3PS_2$
Demetonthiol
Thiophosphorsaeure-*O,O*-diaethyl-*S*-[2-(aethylthio)-aethyl]-ester
O,O-Diethyl-*S*-(2-(ethylthio)-ethyl)ester thiophosphoric acid
RN: 126-75-0 **MP** (°C)**:**
MW: 258.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.742E-03	2.000E+00	20	F300	1 0 0 0 0	

1676. $C_8H_{19}O_4P$
Diethyl butyl phosphate
Butyl diethyl phosphate
RN: 2737-00-0 **MP** (°C)**:**
MW: 210.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.136E-02	1.500E+01	25	B070	1 2 0 1 1	

1677. $C_8H_{19}O_4P$
Diethyl isobutyl phosphate
Ethyl isobutyl phosphate
Phosphoric acid, diethyl 2-methylpropyl ester
RN: 26628-97-7 **MP** (°C)**:**
MW: 210.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-02	1.400E+01	25	B070	1 2 0 1 1	

1678. $C_8H_{19}O_4PS_3$
Disulfoton sulfone
Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester
Disulfoton dioxide
Diethyl *S*-(2-ethylsulfonylethyl) phosphorodithioate
Disyston sulfone
Thiodemeton sulfone
RN: 2497-06-5 **MP** (°C)**:**
MW: 306.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.716E-03	8.323E-01	20	B169	2 2 1 1 1	

1679. $C_8H_{20}Si$
Tetraethylsilicane
Tetraethylsilane
Tetraethylsilicon
RN: 631-36-7 **MP** (°C)**:**
MW: 144.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E-06	3.248E-04	25	D346	0 0 0 0 0	

1680. $C_8H_{20}Sn$
Tetraethyltin
Tetraethylstannane
RN: 597-64-8 **MP** (°C)**:** –112
MW: 234.94 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-06	2.678E-04	25	D346	1 1 2 2 2	

1681. $C_8H_{20}O_5P_2S_2$
Sulfotepp
Pirofos
Tetraethyl dithiopyrophosphate
RN: 3689-24-5 **MP** (°C)**:**
MW: 322.32 **BP** (°C)**:** 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.307E-05	3.000E-02	20	F300	1 0 0 0 0	
7.756E-05	2.500E-02	20	M061	1 0 0 0 1	
7.756E-05	2.500E-02	rt	M161	0 0 0 0 1	

1682. $C_8H_{23}N_5$
Tetraethylenepentamine
1,4,7,10,13-Pentaazatridecane
N-(2-Aminoethyl)-*N′*-(2-((2-aminoethyl)amino)ethyl)-1,2-ethanediamine
1,11-Diamino-3,6,9-triazaundecane
3,6,9-Triaza-1,11-undecanediamine
3,6,9-Triazaundecane-1,11-diamine
RN: 112-57-2 **MP** (°C)**:** –40
MW: 189.31 **BP** (°C)**:** 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.582E+00	8.674E+02	4.50	C022	1 2 0 0 2	

1683. $C_8Cl_4N_2$
Chlorothalonil
2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile
Forturf
Exotherm
Bravo
RN: 1897-45-6 **MP** (°C)**:** 250.5
MW: 265.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.256E-06	6.000E-04	25	M161	1 0 0 0 0	

1684. $C_9H_4Cl_3NO_2S$
Folpet
N-(Trichloromethylthio)phthalimide
Folpan
Folpel
Phaltan
Phalton
RN: 133-07-3 **MP** (°C)**:** 177
MW: 296.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-06	1.005E-03	20	B179	0 0 0 0 0	
3.372E-06	1.000E-03	20	F311	1 2 2 2 1	
3.388E-06	1.005E-03	ns	R427	0 0 0 0 0	

1685. $C_9H_5Cl_3N_4$
Anilazine
4,6-Dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine
Triasyn
Direx
Dyrene
Kemate
RN: 101-05-3 **MP** (°C)**:** 159.5
MW: 275.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.629E-05	1.000E-02	ns	B160	0 0 0 0 1	

1686. $C_9H_6ClNO_3S$
Benazolin
7-Chloro-2-oxo-3(2H)-benzothiazolacetic acid
Galipan
Herbazolin
Leymin
Metizolin
RN: 3813-05-6 **MP** (°C)**:** 193
MW: 243.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	6.000E-01	20	M161	1 0 0 0 2	

1687. $C_9H_6Cl_2N_2O_3$
Methazole
2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione
Tunic
Paxilon
Chlormethazole
Mezopur
RN: 20354-26-1 **MP** (°C)**:** 123
MW: 261.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-06	1.500E-03	24	C105	2 1 2 2 2	
5.746E-06	1.500E-03	25	M161	1 0 0 0 1	
5.746E-06	1.500E-03	25	W314	1 0 0 0 1	

1688. $C_9H_6Cl_6O_3S$
Endosulfan
RN: 115-29-7 **MP** (°C)**:** 209
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.987E-07	3.250E-04	ns	V414	0 0 0 0 0	

1689. $C_9H_6Cl_6O_3S$
α-Endosulfan
5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *endo*-
Endosulfan I
Endosulfan A
Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *endo*-
Thiodan I
RN: 959-98-8 **MP** (°C)**:** 109
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-06	5.099E-04	20	B300	2 0 1 1 2	
1.302E-06	5.300E-04	25	W025	1 0 2 2 2	
4.030E-07	1.640E-04	ns	A069	0 0 0 0 2	
1.253E-06	5.100E-04	ns	V414	0 0 0 0 0	

1690. $C_9H_6Cl_6O_3S$
β-Endosulfan
5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *exo*-
Endosulfan II
Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *exo*-
Thiodan II
RN: 33213-65-9 **MP** (°C)**:** 209
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-06	4.501E-04	20	B300	2 0 1 1 2	
6.881E-07	2.800E-04	25	W025	1 0 2 2 2	
1.720E-07	7.000E-05	ns	A069	0 0 0 0 1	
1.106E-06	4.500E-04	ns	V414	0 0 0 0 0	

1691. $C_9H_6I_3NO_3$
2,4,6-Triiodo-3-acetaminobenzoic acid
Acetrizoic acid
RN: 85-36-9 **MP** (°C)**:**
MW: 556.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-03	1.280E+00	25	L025	1 0 0 0 2	
3.232E-03	1.800E+00	50	L025	1 0 0 0 2	
5.387E-03	3.000E+00	100	L025	1 0 0 0 2	
2.442E-03	1.360E+00	ns	H055	0 0 0 0 0	

1692. $C_9H_6N_2S$
4-Cyanobenzyl isothiocyanate
p-Cyanobenzyl isothiocyanate
Isothiocyanic acid, *p*-cyanobenzyl ester
RN: 3694-48-2 **MP** (°C)**:**
MW: 174.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.575E-02	25	D014	1 0 0 0 1	

1693. $C_9H_6O_2$
Coumarin
Cumarin
1,2-Benzopyrone
2H-1-Benzopyran-2-one
Benzopyran-2-one
Benzopyrone
RN: 91-64-5 **MP** (°C)**:** 70
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.153E-03	8.992E-01	.2	D073	1 1 2 1 0	
8.211E-03	1.200E+00	0	F300	1 0 0 0 1	
1.298E-02	1.896E+00	20	D073	1 1 2 1 1	
1.368E-02	2.000E+00	22.5	G301	0 0 0 0 0	
1.706E-02	2.494E+00	25	I312	0 0 0 0 0	
1.774E-02	2.593E+00	30	D073	1 1 2 1 1	
1.847E-02	2.700E+00	30	F300	1 0 0 0 1	
3.065E-02	4.480E+00	40	D073	1 1 2 1 1	
4.419E-02	6.458E+00	50	D073	1 1 2 1 1	
4.756E-02	6.951E+00	60	D073	1 1 2 1 1	
1.342E-01	1.961E+01	100	I312	0 0 0 0 0	
1.507E-02	2.203E+00	ns	R082	0 0 0 0 0	
6.842E-04	9.999E-02	rt	D021	0 0 1 1 0	*sic*

1694. $C_9H_6O_3$
7-Hydroxycoumarin
Umbelliferone
RN: 93-35-6 **MP** (°C)**:** 230
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	3.110E-01	ns	R082	0 0 0 0 0	

1695. $C_9H_6O_5$
Phthalonic acid
Phthalonsaeure
RN: 528-46-1 **MP** (°C)**:**
MW: 194.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.756E+00	5.350E+02	15	F300	1 0 0 0 2	

1696. $C_9H_6O_6$
Trimesic acid
1,3,5-Benzenetricarboxylic acid
Benzol-tricarbonsaeure-(1,3,5)
RN: 554-95-0 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.808E-02	3.800E+00	16	F300	1 0 0 0 1	
1.252E-01	2.630E+01	23	F300	1 0 0 0 2	

1697. $C_9H_6O_6$
1,2,3-Benzenetricarboxylic acid
Benzol-tricarbonsaeure-(1,2,3)
Hemimellitic acid
RN: 569-51-7 **MP** (°C)**:** 223
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	3.060E+01	19	F300	1 0 0 0 2	

1698. $C_9H_6O_6$
Hydrastic acid
Hydrastsaeure
RN: 490-26-6 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-02	6.000E+00	15	F300	1 0 0 0 1	

1699. $C_9H_7Cl_3O_3$
Trichloroethyl salicylate
Benzoic acid, 2-hydroxy-, 2,2,2-trichloroethyl ester
RN: 56529-85-2 **MP** (°C)**:**
MW: 269.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.081E-03	1.100E+00	37	D009	1 2 1 1 1	0.1N HCl

1700. $C_9H_7Cl_3O_3$
Silvex
2-(2,4,5-Trichlorophenoxy)propionic acid
Fenoprop
Propionic acid, 2(2,4,5-trichlorophenoxy)-
RN: 93-72-1 **MP** (°C)**:** 181.6
MW: 269.51 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	7.088E-02	24.99	N417	0 0 0 0 0	
2.634E-04	7.100E-02	25	B164	1 0 1 1 1	
5.195E-04	1.400E-01	25	B185	0 0 0 0 0	
6.678E-04	1.800E-01	25	B200	1 0 0 0 1	
5.195E-04	1.400E-01	25	L024	1 0 0 0 2	
5.194E-04	1.400E-01	25	M061	1 0 0 0 1	
5.195E-04	1.400E-01	25	M161	1 0 0 0 2	
5.194E-04	1.400E-01	ns	B100	0 0 0 0 1	
5.195E-04	1.400E-01	ns	K138	0 0 0 0 1	

1701. C_9H_7N
Quinoline
Chinolin
1-Azanaphthalene
Benzopyridine
1-Benzazine
Benzo[b]pyridine
RN: 91-22-5 **MP** (°C)**:** –15
MW: 129.16 **BP** (°C)**:** 237.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.730E-02	6.110E+00	20	A050	0 0 0 0 0	
4.913E-02	6.346E+00	20.3	L339	2 0 2 2 2	
4.968E-02	6.417E+00	40.0	L339	2 0 2 2 2	
6.337E-02	8.185E+00	64.8	L339	2 0 2 2 2	
8.136E-02	1.051E+01	80.2	L339	2 0 2 2 2	
1.063E-01	1.373E+01	100.0	L339	2 0 2 2 2	

1702. C_9H_7NO
4-Hydroxyquinoline
4-Hydroxy-chinolin
4-Quinolinol
RN: 611-36-9 **MP** (°C)**:** 201
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-02	4.800E+00	15	F300	1 0 0 0 1	

1703. C_9H_7NO
5-Hydroxyquinoline
5-Quinolinol
RN: 578-67-6 **MP** (°C)**:** 223
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.869E-03	4.165E-01	20	A035	1 0 2 2 1	
2.884E-03	4.187E-01	ns	R427	0 0 0 0 0	

1704. C_9H_7NO
6-Hydroxyquinoline
6-Quinolinol
RN: 580-16-5 **MP** (°C)**:** 192
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.882E-03	9.990E-01	20	A035	1 0 2 2 1	

1705. C_9H_7NO
7-Hydroxyquinoline
7-Quinolinol
RN: 580-20-1 **MP** (°C)**:**
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	4.543E-01	20	A035	1 0 2 2 1	
3.162E-03	4.590E-01	ns	R427	0 0 0 0 0	

1706. C_9H_7NO
8-Hydroxyquinoline
8-Quinolinol
Hydroxybenzopuridine
RN: 148-24-3 **MP** (°C)**:** 76
MW: 145.16 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-03	5.552E-01	20	A035	1 0 2 2 1	
4.470E-03	6.489E-01	25.2	P024	2 1 1 1 2	
5.380E-03	7.810E-01	30.3	P024	2 1 1 1 2	

1707. C_9H_7NO
Carbostyril
2-Hydroxyquinoline
2-Quinolinol
RN: 59-31-4 **MP** (°C)**:** 199.0
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.244E-03	1.052E+00	20	C035	1 0 2 2 1	

1708. C_9H_7NO
3-Hydroxyquinoline
3-Quinolinol
RN: 580-18-7 **MP** (°C)**:**
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-03	5.879E-01	20	A035	1 0 2 2 1	

1709. C_9H_7NOS
m-Acetylphenyl isothiocyanate
3-Acetylphenyl isothiocyanate
RN: 3125-71-1 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-05	8.330E-03	25	K032	2 2 0 1 1	

1710. C_9H_7NOS
p-Acetylphenyl isothiocyanate
4-Acetylphenyl isothiocyanate
RN: 2131-57-9 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-05	1.684E-02	25	D019	1 1 1 1 1	

1711. C_9H_7NOS
Phenacyl thiocyanate
RN: 5399-30-4 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-03	3.494E-01	22	J420	0 0 0 0 0	pH 6.5

1712. $C_9H_7NO_2S$
m-Acetoxyphenyl isothiocyanate
Methyl *m*-isothiocyanobenzoate
RN: 3530-01-6 **MP** (°C)**:**
MW: 193.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-04	5.256E-02	25	K032	2 2 0 1 2	
7.700E-04	1.488E-01	25	K032	2 2 0 1 2	

1713. $C_9H_7NO_5$
2-(Oxalylamino)benzoic acid
Oxanil-carbonsaeure-(2)
Oxanil-*o*-carboxylic acid
RN: 5651-01-4 **MP** (°C)**:**
MW: 209.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.259E-03	1.100E+00	10	F300	1 0 0 0 1	

1714. $C_9H_7N_3S$
Tricyclazole
Methyl-1,2,4-triazolo(3,4-b)benzothiazole
5-Methyl-1,2,4-triazolo[3,4-b]benzothiazole
RN: 41814-78-2 **MP** (°C)**:** 187.5
MW: 189.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-03	1.600E+00	25	M161	1 0 0 0 1	

1715. $C_9H_7N_7O_2S$
Azathioprine
Cytostatics
Imuran
Azatioprin
6-(1-Methyl-*p*-nitro-5-imidazolyl)-thiopurine
Ccucol
RN: 446-86-6 **MP** (°C)**:** 243.5
MW: 277.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-04	1.300E-01	24	N016	0 0 0 0 0	
4.472E-04	1.240E-01	25	N063	1 1 1 1 2	intrinsic
4.689E-04	1.300E-01	25	N063	1 1 1 1 2	
3.607E-05	1.000E-02	ns	K444	0 0 0 0 0	

1716. $C_9H_8Cl_2O_3$
Dichlorprop
Dichloroprop
α-(2,4-Dichlorophenoxy)propionic acid
RN: 120-36-5 **MP** (°C)**:** 117.5
MW: 235.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.489E-03	3.500E-01	20	L024	1 0 0 0 2	
1.489E-03	3.500E-01	20	M161	1 0 0 0 2	
1.490E-03	3.503E-01	24.99	N417	0 0 0 0 0	
3.527E-03	8.290E-01	25	B164	1 0 1 1 2	
3.020E-03	7.100E-01	28	B200	1 0 0 0 1	
1.484E-02	3.488E+00	ns	B100	0 0 0 0 1	

1717. $C_9H_8Cl_2O_3$
Methyl (2,4-Dichlorophenoxy)acetate
2,4-Dichorophenoxyacetic acid methyl ester
RN: 5335-03-5 **MP** (°C)**:**
MW: 235.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.657E-04	1.800E-01	ns	B185	0 0 0 0 0	
5.333E-04	1.254E-01	ns	M120	0 0 1 1 2	

1718. $C_9H_8Cl_3NO_2S$
Captan
N-Trichloromethylthio-4-cyclohexene-1,2-dicarboximide
Vancide 89
Merpan 90
Orthocid-83
Pillarcap
RN: 133-06-2 **MP** (°C)**:** 178
MW: 300.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-06	4.989E-04	20	B179	0 0 0 0 0	
<1.66E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.544E-05	4.642E-03	ns	H322	0 0 0 0 0	
1.660E-06	4.989E-04	ns	R427	0 0 0 0 0	
1.663E-06	5.000E-04	rt	M161	0 0 0 0 0	

1719. $C_9H_8N_2OS$
m-Acetamidophenyl isothiocyanate
3-Acetamidophenyl isothiocyanate
RN: 3137-83-5 **MP** (°C)**:**
MW: 192.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.950E-04	5.671E-02	25	K032	2 2 0 1 2	

1720. $C_9H_8N_4O_6$
Nifurtoinol
3-(Hydroxymethyl)nitrofurantoin
RN: 1088-92-2 **MP** (°C)**:**
MW: 268.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	3.300E-01	22	B154	1 1 1 1 1	0.1M HCl

1721. C_9H_8O
(E)-Cinnamaldehyde
(E)-3-Phenylpropenal;
(2E)-3-Phenyl-2-propenal
(E)-3-Phenylprop-2-enone
(E)-3-Phenylacrolein
(E)-3-Phenylprop-2-enal
RN: 14371-10-9 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:** 250–253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	1.850E+00	25	D407	1 0 2 2 2	

1722. C_9H_8O
Cinnamaldehyde
3-Phenyl-2-propenal
Phenylacrolein
3-Phenyl-2-propenaldehyde
Zimtaldehyde
RN: 104-55-2 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.348E+00	25	I019	1 0 1 2 2	
9.100E-03	1.203E+00	37	E028	1 0 1 1 1	

1723. $C_9H_8O_2$
trans-Cinnamic acid
trans-3-Phenyl-2-propenoic acid
trans-β-Phenylacrylic acid
(E)-3-Phenyl-2-propenoic acid
RN: 140-10-3 **MP** (°C)**:** 133
MW: 148.16 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-03	2.100E-01	15	M461	0 0 0 0 0	
2.700E-03	4.000E-01	18	F300	1 0 0 0 0	
2.835E-03	4.200E-01	18	M077	1 2 1 1 2	
3.010E-03	4.460E-01	25	C090	1 2 2 2 2	
3.685E-03	5.460E-01	25	M077	1 2 1 1 2	
1.552E-03	2.300E-01	25	M461	0 0 0 0 0	
2.092E-03	3.100E-01	30	M461	0 0 0 0 0	
5.264E-03	7.800E-01	35	M077	1 2 1 1 2	
4.252E-03	6.300E-01	40	M461	0 0 0 0 0	
7.364E-03	1.091E+00	45	M077	1 2 1 1 2	
5.737E-03	8.500E-01	50	M461	0 0 0 0 0	

1724. $C_9H_8O_2$
Atropic acid
Atropasaeure
RN: 492-38-6 **MP** (°C)**:** 106
MW: 148.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.774E-03	1.300E+00	20	F300	1 0 0 0 1	

1725. $C_9H_8O_2$
Cinnamic acid
Phenylacrylic acid
3-Phenylpropenoic acid
2-Propenoic acid, 3-phenyl-
RN: 621-82-9 **MP** (°C)**:** 133
MW: 148.16 **BP** (°C)**:** 261.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.024E-03	2.999E-01	10	M043	1 0 0 0 0	
3.390E-03	5.023E-01	14.3	D061	1 0 0 0 2	
2.642E-03	3.914E-01	16.3	D061	1 0 0 0 2	
2.643E-03	3.916E-01	16.30	B118	1 0 0 0 2	unit assumed
1.515E-02	2.245E+00	20	C092	2 1 0 1 1	*sic*
2.699E-03	3.998E-01	20	M043	1 0 0 0 0	
3.170E-03	4.697E-01	22	E045	2 0 1 1 2	
3.260E-03	4.830E-01	23	E045	2 0 1 1 2	
3.360E-03	4.978E-01	24	E045	2 0 1 1 2	
3.450E-03	5.112E-01	25	E045	2 0 1 1 2	
3.850E-03	5.704E-01	25	K040	1 0 2 1 2	
3.340E-03	4.949E-01	25	L048	1 2 2 1 2	
3.340E-03	4.949E-01	25	L050	2 0 1 2 2	
3.540E-03	5.245E-01	26	E045	2 0 1 1 2	
3.800E-03	5.630E-01	26.4	P043	2 0 1 1 2	
3.630E-03	5.378E-01	27	E045	2 0 1 1 2	
4.963E-03	7.353E-01	28	D050	1 2 1 2 2	
4.688E-03	6.946E-01	30	B118	1 0 0 0 2	unit assumed
4.682E-03	6.937E-01	30	D061	1 0 0 0 2	
4.047E-03	5.996E-01	30	M043	1 0 0 0 0	
3.959E-02	5.865E+00	100	M043	1 0 0 0 1	

1726. $C_9H_8O_2$
cis-Cinnamic acid
cis-Zimtsaeure
RN: 102-94-3 **MP** (°C)**:**
MW: 148.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.657E-02	6.900E+00	18	F300	1 0 0 0 1	
4.644E-02	6.880E+00	18	M077	1 2 1 1 2	form III, mp 68 C
5.143E-02	7.620E+00	18	M077	1 2 1 1 2	form II, mp 58 C
6.041E-02	8.950E+00	18	M077	1 2 1 1 2	form I, mp 42 C
5.703E-02	8.450E+00	25	M077	1 2 1 1 2	form III, mp 68 C
6.324E-02	9.370E+00	25	M077	1 2 1 1 2	form II, mp 58 C
7.445E-02	1.103E+01	25	M077	1 2 1 1 2	form I, mp 42 C
7.519E-02	1.114E+01	35	M077	1 2 1 1 2	form III, mp 68 C
8.362E-02	1.239E+01	35	M077	1 2 1 1 2	form II, mp 58 C

(*continued*)

1726. $C_9H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.861E-02	1.461E+01	35	M077	1 2 1 1 2	form I, mp 42 C
9.760E-02	1.446E+01	45	M077	1 2 1 1 2	form III, mp 68 C
1.086E-01	1.609E+01	45	M077	1 2 1 1 2	form II, mp 58 C
1.245E-01	1.845E+01	55	M077	1 2 1 1 2	form III, mp 68 C

1727. $C_9H_8O_3$
2-Acetophenone carboxylic acid
Acetophenon-carbonsaeure-(2)
o-Carboxyacetophenone
RN: 577-56-0 **MP** (°C)**:**
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	3.984E+00	rt	H431	0 0 0 0 0	

1728. $C_9H_8O_4$
Homophthalic acid
Homophthalsaeure
RN: 89-51-0 **MP** (°C)**:** 184.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-02	4.579E+00	rt	H431	0 0 0 0 0	

1729. $C_9H_8O_4$
Caffeic acid
3,4-Dihydroxy-*trans*-cinnamate
(E)-3-(3,4-Dihydroxyphenyl)-2-propenoic acid
RN: 331-39-5 **MP** (°C)**:** 196 C
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-03	5.500E-01	15	M461	0 0 0 0 0	
5.440E-03	9.800E-01	25	M461	0 0 0 0 0	
6.827E-03	1.230E+00	30	M461	0 0 0 0 0	
1.132E-02	2.040E+00	40	M461	0 0 0 0 0	
1.621E-02	2.920E+00	50	M461	0 0 0 0 0	

1730. $C_9H_8O_4$
4-Methylphthalic acid
RN: 4316-23-8 **MP** (°C)**:** 149
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.211E-02	3.984E+00	rt	H431	0 0 0 0 0	

1731. $C_9H_8O_4$
Aspirin
Acetyl-salicylsaeure
Acetylsalicylic acid
RN: 50-78-2 **MP** (°C)**:** 135
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-02	5.623E+00	4.62	M053	1 0 1 1 0	EFG, 0.1N HCl
1.107E-02	1.995E+00	12.55	M053	1 0 1 1 0	EFG, 0.1N HCl
3.200E-02	5.765E+00	14	O019	1 0 0 1 2	
1.998E-02	3.600E+00	15	E017	1 0 0 0 0	EFG
1.388E-02	2.500E+00	15	F300	1 0 0 0 1	
1.716E-02	3.091E+00	15	H022	1 2 2 2 2	
2.109E-02	3.800E+00	20	E017	1 0 0 0 0	EFG
1.460E-02	2.630E+00	20.96	M053	1 0 1 1 0	EFG, 0.1N HCl
1.769E-02	3.188E+00	22.5	B422	2 0 2 2 2	
2.553E-02	4.600E+00	25	E017	1 0 0 0 0	EFG
2.775E-02	5.000E+00	25	S304	1 2 1 2 2	form IV
2.131E-02	3.840E+00	25	S304	1 2 1 2 2	form I
2.442E-02	4.400E+00	25	S304	1 2 1 2 2	form II
1.890E-02	3.405E+00	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.62, intrinsic
2.500E-02	4.504E+00	30	A065	2 0 2 2 1	
2.831E-02	5.100E+00	30	E017	1 0 0 0 0	EFG
2.387E-02	4.300E+00	30	G042	1 1 1 1 1	0.1N HCl
2.851E-02	5.137E+00	30	H022	1 2 2 2 2	
2.000E-02	3.603E+00	30	L069	1 0 1 1 0	EFG
2.637E-02	4.750E+00	30	S304	1 2 1 2 2	form I
3.275E-02	5.900E+00	30	S304	1 2 1 2 2	form IV
3.108E-02	5.600E+00	30	S304	1 2 1 2 2	form II
3.275E-02	5.900E+00	35	E017	1 0 0 0 0	EFG
2.942E-02	5.300E+00	37	D009	1 2 1 1 1	0.1N HCl
3.219E-02	5.800E+00	37	G042	1 1 1 1 1	0.1N HCl
3.641E-02	6.560E+00	37	G430	0 0 0 0 0	pH 4.5
3.569E-02	6.430E+00	37	K086	1 0 0 0 2	
3.031E-02	5.460E+00	37	M115	2 2 1 1 2	
4.052E-02	7.300E+00	37	S304	1 2 1 2 2	form II
3.830E-02	6.900E+00	37	S304	1 2 1 2 2	form I
4.218E-02	7.600E+00	37	S304	1 2 1 2 2	form IV
3.441E-02	6.200E+00	37	Y421	0 0 0 0 0	

(*continued*)

1731. $C_9H_8O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	6.900E+00	40	E017	1 0 0 0 0	EFG
4.385E-02	7.900E+00	40	S304	1 2 1 2 2	form II
4.218E-02	7.600E+00	40	S304	1 2 1 2 2	form I
4.607E-02	8.300E+00	40	S304	1 2 1 2 2	form IV
4.662E-02	8.400E+00	45	E017	1 0 0 0 0	EFG
4.274E-02	7.700E+00	45	G042	1 1 1 1 1	0.1N HCl
5.551E-02	1.000E+01	49.42	M053	1 0 1 1 0	EFG, 0.1N HCl
4.940E-02	8.900E+00	50	G042	1 1 1 1 1	0.1N HCl
6.829E-02	1.230E+01	60.17	M053	1 0 1 1 0	EFG, 0.1N HCl
1.848E-02	3.330E+00	ns	K444	0 0 0 0 0	
1.551E-02	2.795E+00	rt	R431	0 0 0 0 0	Average

1732. $C_9H_9ClO_3$

DL-2-(2-Chlorophenoxy)propionic acid
2-(*o*-Chlorophenoxy)propionic acid
3-CP

RN: 76466-16-5 **MP** (°C)**:** 113
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.974E-03	1.199E+00	22	B200	1 0 0 0 1	
9.726E-02	1.951E+01	100	B200	1 0 0 0 2	

1733. $C_9H_9ClO_3$

DL-2-(4-Chlorophenoxy)propionic acid

RN: 3307-39-9 **MP** (°C)**:**
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.352E-03	1.475E+00	25	B164	1 0 1 1 2	
7.352E-03	1.475E+00	25	B185	0 0 0 0 0	

1734. $C_9H_9ClO_3$

(4-Chloro-2-methylphenoxy)acetic acid
MCPA

RN: 94-74-6 **MP** (°C)**:** 120.0
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	6.296E-01	20	M061	1 0 0 0 1	
5.852E-03	1.174E+00	25	B164	1 0 1 1 2	
5.852E-03	1.174E+00	25	B185	0 0 0 0 0	
7.975E-03	1.600E+00	25	B185	0 0 0 0 0	

(*continued*)

1734. $C_9H_9ClO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.979E-03	9.990E-01	ns	B100	0 0 0 0 0	
3.190E-03	6.400E-01	ns	B185	0 0 0 0 0	
4.112E-03	8.250E-01	ns	L024	0 0 0 0 2	
4.112E-03	8.250E-01	rt	M161	0 0 0 0 2	

1735. $C_9H_9Cl_2NO$

Propanil
3′,4′-Dichloropropionanilide
DPA

RN: 709-98-8 **MP** (°C)**:** 85
MW: 218.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.961E-04	1.300E-01	20	F311	1 2 2 2 1	
2.293E-03	5.000E-01	ns	B185	0 0 0 0 0	
2.292E-03	4.998E-01	ns	B200	0 0 0 0 0	
2.293E-03	5.000E-01	ns	H042	0 0 0 0 2	
1.032E-03	2.250E-01	rt	M161	0 0 0 0 2	

1736. $C_9H_9Cl_2NO_2$

Dichlormate
3,4-Dichlorobenzyl *N*-methylcarbamate
Romate

RN: 1966-58-1 **MP** (°C)**:** 52
MW: 234.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	25	B200	1 0 0 0 2	

1737. $C_9H_9Cl_2NO_2$

UC 22463
Sirmate 4E
Rowmate
Sirmate

RN: 62046-37-1 **MP** (°C)**:** 52
MW: 234.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	ns	H042	0 0 0 0 2	

1738. $C_9H_9I_2NO_3$
L-3,5-Diiodotyrosine
3,5-Diiodo-L-tyrosine
DIT
RN: 300-39-0 **MP** (°C)**:** 213
MW: 432.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-03	6.196E-01	25	D041	1 0 0 0 1	

1739. $C_9H_9I_2NO_3$
3,5-Diiodotyrosine
3,5-Diiod-DL-tyrosin
DL-Thyronin
RN: 66-02-4 **MP** (°C)**:** 204
MW: 432.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-03	4.500E-01	15	F300	1 0 0 0 1	
7.850E-04	3.399E-01	25	D041	1 0 0 0 1	
1.386E-03	6.000E-01	25	F300	1 0 0 0 0	
1.316E-02	5.700E+00	75	F300	1 0 0 0 1	

1740. C_9H_9N
Skatole
3-Methyl-indol
3-Methylindole
RN: 83-34-1 **MP** (°C)**:** 95
MW: 131.18 **BP** (°C)**:** 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-03	4.500E-01	16	F300	1 0 0 0 0	

1741. C_9H_9NOS
m-Ethoxyphenyl isothiocyanate
3-Ethoxyphenyl isothiocyanate
RN: 3701-44-8 **MP** (°C)**:**
MW: 179.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-04	6.811E-02	25	K032	2 2 0 1 2	

1742. C_9H_9NOS
p-Ethoxyphenyl isothiocyanate
4-Ethoxyphenyl isothiocyanate
RN: 25687-50-7 **MP** (°C)**:**
MW: 179.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	9.858E-03	25	D019	1 1 1 1 1	

1743. $C_9H_9NO_2$
p-Acetamidobenzaldehyde
Acetamide, *N*-(4-formylphenyl)-
Acetanilide, 4′-formyl-
Micotiazone
RN: 122-85-0 **MP** (°C)**:**
MW: 163.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-02	3.247E+00	25	D044	0 0 0 0 0	

1744. $C_9H_9NO_3$
Hippuric acid
Hippursaeure
N-Benzoylglycine
Benzoylaminoacetic acid
RN: 495-69-2 **MP** (°C)**:** 187
MW: 179.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	3.289E+00	20	D041	1 0 0 0 1	
2.177E-02	3.900E+00	20	F300	1 0 0 0 1	
2.050E-02	3.673E+00	25	B028	1 0 0 0 2	
2.048E-02	3.670E+00	25	K053	2 2 2 2 2	
2.095E-02	3.754E+00	25	L048	1 2 2 1 2	
2.095E-02	3.754E+00	25	L050	2 0 1 2 2	
2.048E-02	3.670E+00	25.1	N026	0 0 0 0 0	
3.320E-02	5.949E+00	38	B028	1 0 0 0 2	
2.334E-02	4.182E+00	rt	D021	0 0 1 1 1	

1745. $C_9H_9NO_3$
Acetamide, 2-(benzoyloxy)-
Glycolamide, benzoate
RN: 64649-43-0 **MP** (°C)**:** 121
MW: 179.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.288E-02	4.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
2.288E-02	4.100E+00	22	N317	1 1 2 1 2	

1746. $C_9H_9NO_4$
Benzadox
((Benzoylamino)oxy)acetic acid
Topcide
RN: 5251-93-4 **MP** (°C)**:**
MW: 195.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.069E-02	1.575E+01	ns	B100	0 0 0 0 1	

1747. C_9H_9NS
p-Methylbenzyl isothiocyanate
4-Methylbenzyl isothiocyanate
RN: 3694-46-0 **MP** (°C)**:**
MW: 163.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	2.612E-02	25	D014	1 0 0 0 1	

1748. $C_9H_9N_3OS$
Benzthiazuron
Benzothiazol-2-yl-3-methylurea
N-2-Benzothiazolyl-*N′*-methylurea
Gatnon
RN: 1929-88-0 **MP** (°C)**:**
MW: 207.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-05	1.200E-02	20	M161	1 0 0 0 1	

1749. $C_9H_9N_3O_2$
Carbendazim
1H-Benzimidazol-2-ylcarbamic acid methyl ester
RN: 10605-21-7 **MP** (°C)**:** 302
MW: 191.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-05	5.800E-03	20	A064	1 0 1 1 1	
3.034E-05	5.800E-03	20	M161	1 0 0 0 1	pH 7

1750. $C_9H_9N_3O_2S_2$
Sulfathiazole
Sulphathiazole
*N*1-2-Thiazolyl-
4-Amino-*N*-2-thiazolyl-
RN: 72-14-0 **MP** (°C)**:** 202
MW: 255.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-03	3.600E-01	16	H114	1 0 0 0 1	
1.743E-03	4.450E-01	20	F073	1 2 2 2 2	
1.958E-03	5.000E-01	20	F074	1 0 0 0 2	
4.426E-03	1.130E+00	20	K028	2 1 2 1 2	pH 7.3, form I
1.414E-03	3.610E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.460E-03	6.280E-01	20	K028	2 1 2 1 2	pH 7.3, form II
2.483E-03	6.340E-01	20	K028	2 1 2 1 2	pH 3.8, form I
1.347E-03	3.439E-01	20	L058	1 0 1 1 1	
2.482E-03	6.336E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 200–202 C
1.413E-03	3.609E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 175 C
1.305E-03	3.332E-01	25	F415	0 0 0 0 0	Average
1.461E-03	3.730E-01	25	H005	1 0 1 2 2	average of 4
1.821E-03	4.650E-01	25	K096	1 2 2 2 2	α form
3.290E-03	8.400E-01	25	K096	1 2 2 2 2	β form
1.796E-03	4.586E-01	25	M440	0 0 0 0 0	
1.966E-03	5.020E-01	26	C102	2 0 2 2 2	
2.350E-03	6.000E-01	26	L052	1 0 0 0 0	
2.270E-03	5.796E-01	30	H018	0 0 0 0 0	
4.308E-03	1.100E+00	30	K096	1 2 2 2 2	β form
2.327E-03	5.940E-01	30	K096	1 2 2 2 2	α form
2.544E-03	6.496E-01	30	M046	1 0 0 0 1	
4.460E-03	1.139E+00	30.0	H010	2 2 1 1 2	
3.564E-03	9.100E-01	35	H114	1 0 0 0 1	
3.094E-03	7.900E-01	35	K096	1 2 2 2 2	α form
5.354E-03	1.367E+00	35	K096	1 2 2 2 2	β form
3.760E-03	9.600E-01	37	C102	2 0 2 2 2	
3.564E-03	9.100E-01	37	D084	1 0 1 0 1	
3.678E-03	9.391E-01	37	F072	1 0 0 0 2	

(*continued*)

1750. $C_9H_9N_3O_2S_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-03	9.411E-01	37	F075	1 0 2 2 2	
3.443E-03	8.790E-01	37	K091	1 0 0 0 2	
2.560E-03	6.536E-01	37	K095	2 0 0 0 2	intrinsic
3.838E-03	9.800E-01	37	L091	1 0 0 0 1	pH 5.5
3.721E-03	9.500E-01	37	M057	1 0 0 0 2	pH 5.5
3.799E-03	9.700E-01	37	R044	0 0 0 0 0	
3.756E-03	9.591E-01	37.50	M142	1 0 0 0 1	
3.603E-03	9.200E-01	38	K006	1 0 0 0 2	
6.619E-03	1.690E+00	40	K096	1 2 2 2 2	β form
4.073E-03	1.040E+00	40	K096	1 2 2 2 2	α form
8.284E-03	2.115E+00	45	K096	1 2 2 2 2	β form
5.288E-03	1.350E+00	45	K096	1 2 2 2 2	α form
6.592E-03	1.683E+00	49	K096	1 2 2 2 2	α form
9.964E-03	2.544E+00	49	K096	1 2 2 2 2	β form
1.683E-03	4.298E-01	ns	L044	0 0 0 0 2	
3.467E-03	8.853E-01	ns	R427	0 0 0 0 0	
1.918E-03	4.898E-01	rt	N015	0 0 2 2 2	

1751. C_9H_{10}
Indan
2,3-Dihydroindene
Hydrindane
1H-Indene, 2,3-dihydro-
Hydrindene
RN: 496-11-7 **MP** (°C)**:** –51.4
MW: 118.18 **BP** (°C)**:** 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.232E-04	1.091E-01	25	M064	1 1 2 2 2	
7.522E-04	8.890E-02	25	P051	2 1 1 2 2	
9.232E-04	1.091E-01	ns	M344	0 0 0 0 2	

1752. C_9H_{10}
α-Methylstyrene
2-Phenyl-1-propene
Isopropenylbenzene
2-Phenylpropene
β-Phenylpropene
RN: 98-83-9 **MP** (°C)**:** –24.0
MW: 118.18 **BP** (°C)**:** 167.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-04	1.155E-01	ns	D001	0 0 0 0 2	

1753. $C_9H_{10}BrClN_2O_2$

Chlorbromuron
3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea
N′-(4-Bromo-3-chlorophenyl)-*N*-methoxy-*N*-methylurea
Maloran
RN: 13360-45-7 **MP** (°C)**:**
MW: 293.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.529E-02	20	B179	0 0 0 0 0	
1.192E-04	3.500E-02	20	M161	1 0 0 0 1	
1.703E-04	5.000E-02	ns	B200	0 0 0 0 1	
1.703E-04	5.000E-02	ns	G036	0 0 0 0 1	

1754. $C_9H_{10}Cl_2N_2O$

Diuron
1,1-Dimethyl-3-(3,4-dichlorophenyl)urea
3-(3,4-Dichlorophenyl)-1,1-dimethylurea
RN: 330-54-1 **MP** (°C)**:** 158
MW: 233.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	4.242E-02	20	B179	0 0 0 0 0	
9.438E-05	2.200E-02	20	E048	1 2 1 1 1	
1.716E-04	4.000E-02	25	A039	1 1 0 0 2	
1.802E-04	4.200E-02	25	B185	0 0 0 0 0	
1.802E-04	4.200E-02	25	B200	1 0 0 0 1	
1.802E-04	4.200E-02	25	G036	1 0 0 0 1	
1.802E-04	4.200E-02	25	G099	1 0 0 1 0	
1.600E-04	3.730E-02	25	H073	2 1 1 2 2	
1.802E-04	4.200E-02	25	M061	1 0 0 0 1	
1.802E-04	4.200E-02	25	M161	1 0 0 0 1	
1.802E-04	4.200E-02	25	N333	0 0 0 0 0	
1.716E-04	4.000E-02	ns	B160	0 0 0 0 1	
1.802E-04	4.200E-02	ns	H042	0 0 0 0 1	
1.000E+02	2.331E+04	ns	H342	0 0 0 0 0	EFG, *sic*
1.802E-04	4.200E-02	ns	K007	0 0 0 0 1	
1.995E-04	4.651E-02	ns	M163	0 0 0 0 0	EFG
1.802E-04	4.200E-02	ns	V414	0 0 0 0 0	

1755. $C_9H_{10}Cl_2N_2O_2$

Linuron
3-(3,4-Dichlorophenyl)-1-methoxy-1-methylurea
RN: 330-55-2 **MP** (°C)**:** 93
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-04	7.523E-02	20	B179	0 0 0 0 0	
3.011E-04	7.500E-02	25	B185	0 0 0 0 0	

(*continued*)

1755. $C_9H_{10}Cl_2N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-04	7.500E-02	25	B200	1 0 0 0 1	
3.011E-04	7.500E-02	25	M061	1 0 0 0 1	
3.011E-04	7.500E-02	25	M161	1 0 0 0 1	
3.252E-04	8.100E-02	25	M162	1 1 0 0 1	
3.011E-04	7.500E-02	ns	K007	0 0 0 0 1	

1756. $C_9H_{10}Cl_2O$

2,4-Dichloro-6-propyl-phenol
RN: 91399-12-1 **MP** (°C)**:**
MW: 205.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.005E-01	25	B316	0 0 0 0 0	

1757. $C_9H_{10}Cl_3O_3PS$

Trichlormetafos-3
O-Methyl *O*-ethyl *O*-2,4,5-trichlorophenyl thiophosphate
RN: 2633-54-7 **MP** (°C)**:**
MW: 335.58 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.19E-04	<4.00E-02	ns	M061	0 0 0 0 0	

1758. $C_9H_{10}NO_3$

2-Oxo-5-indolinyl acetate
5-Acetoxy-2-oxindole
RN: 74973-14-1 **MP** (°C)**:**
MW: 180.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	5.225E+00	25	A066	1 0 1 1 1	

1759. $C_9H_{10}NO_3PS$

Cyanophos
Dimethyl *O*-(*p*-cyanophenyl) phosphorothioate
Ciafos
CYAP
RN: 2636-26-2 **MP** (°C)**:** 14.5
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.891E-04	4.600E-02	30	M161	1 0 0 0 1	

1760. $C_9H_{10}N_2O_2$
Phenacemide
Phenylacetyl urea
RN: 63-98-9 **MP** (°C)**:** 215
MW: 178.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E-03	1.820E-01	ns	B404	0 2 1 1 0	

1761. $C_9H_{10}N_2O_3$
p-Nitroacetotoluide
4-Nitroacetotoluide
RN: **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1762. $C_9H_{10}N_2O_3$
p-Ureidophenyl acetate
4-Ureidophenyl acetate
RN: 59746-11-1 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-03	6.214E-01	25	A066	1 0 1 1 1	

1763. $C_9H_{10}N_2O_3$
o-Nitroacetotoluide
2-Nitroacetotoluide
RN: 612-45-3 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1764. $C_9H_{10}N_2O_3S_2$
Ethoxzolamide
6-Ethoxy-2-benzothiazolesulfonamide
Diuretic C
Cardrase
RN: 452-35-7 **MP** (°C)**:** 188
MW: 258.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.033E-02	25	C415	1 0 0 1 0	
1.548E-04	4.000E-02	ns	M032	0 0 0 0 0	
1.549E-04	4.001E-02	ns	R428	0 0 0 0 0	

1765. $C_9H_{10}N_2S$
4-Dimethylaminophenyl isothiocyanate
4-Isothiocyanato-*N,N*-dimethyl-benzenamine
RN: 2131-64-8 **MP** (°C)**:**
MW: 178.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-05	1.337E-02	25	D019	1 1 1 1 1	

1766. $C_9H_{10}N_2S$
3-Dimethylaminophenyl isothiocyanate
N′,N′-Dimethyl-*m*-aminophenyl isothiocyanate
RN: 2392-67-8 **MP** (°C)**:**
MW: 178.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-04	7.487E-02	25	D019	1 1 1 1 2	
1.950E-04	3.476E-02	25	K032	2 2 0 1 2	

1767. $C_9H_{10}N_4$
2,6,7-Trimethylpteridine
2:6:7-Trimethylpteridine
RN: 23767-00-2 **MP** (°C)**:**
MW: 174.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.087E-02	1.235E+01	20	A083	1 2 0 0 0	

1768. $C_9H_{10}N_4O_2S_2$
Sulfamethizole
Sulfamethylthiadiazole
RN: 144-82-1 **MP** (°C)**:** 208
MW: 270.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.957E-03	5.290E-01	20	F073	1 2 2 2 2	
3.320E-03	8.975E-01	37	A046	2 0 1 1 2	
3.884E-03	1.050E+00	37	B046	1 0 2 2 2	pH 4.5
3.270E-03	8.840E-01	37	K091	1 0 0 0 2	
3.270E-03	8.840E-01	37	W016	2 0 1 1 2	
2.938E-03	7.943E-01	ns	N057	1 0 2 2 0	EFG, intrinsic

1769. $C_9H_{10}O$
Propiophenone
1-Phenyl-1-propanone
Ethyl phenyl ketone
Propiophenoe
RN: 93-55-0 **MP** (°C)**:** 19
MW: 134.18 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-02	1.985E+00	ns	S460	0 0 0 0 0	

1770. $C_9H_{10}O_2$
Hydrocinnamic acid
Hydrozimtsaeure
RN: 501-52-0 **MP** (°C)**:** 48
MW: 150.18 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.929E-02	5.900E+00	20	F300	1 0 0 0 2	
6.162E-02	9.254E+00	30	D033	2 2 1 2 2	
7.668E-02	1.152E+01	40	D033	2 2 1 2 2	

1771. $C_9H_{10}O_2$
2,5-Dimethylbenzoic acid
2-Carboxy-1,4-dimethylbenzene
Isoxylic acid
RN: 610-72-0 **MP** (°C)**:** 132.5–134.5
MW: 150.18 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-03	1.800E-01	25	H007	0 0 0 0 0	

1772. $C_9H_{10}O_2$
2,4-Dimethylbenzoic acid
4-Carboxy-1,3-dimethylbenzene
RN: 611-01-8 **MP** (°C)**:** 124–126
MW: 150.18 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.065E-03	1.600E-01	25	H007	0 0 0 0 0	

1773. $C_9H_{10}O_2$
Benzyl acetate
Phenylmethyl acetate
Acetic acid phenylmethyl ester
α-Acetoxytoluene
RN: 140-11-4 **MP** (°C)**:** –51.3
MW: 150.18 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.973E-03	1.498E+00	25	M350	1 0 1 1 1	

1774. $C_9H_{10}O_2$
3,4-Dimethylbenzoic acid
1-Carboxy-3,4-dimethylbenzene
RN: 619-04-5 **MP** (°C)**:** 165
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-04	1.292E-01	ns	C014	0 0 0 1 1	

1775. $C_9H_{10}O_2$
Ethyl benzoate
Ethyl *p*-benzoate
Benzoesaeure-aethyl ester
RN: 93-89-0 **MP** (°C)**:** –34
MW: 150.18 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.990E-03	1.200E+00	22	N317	1 1 2 1 2	
4.794E-03	7.200E-01	25	A003	1 2 1 2 1	
6.659E-03	1.000E+00	60	F300	1 0 0 0 0	

1776. $C_9H_{10}O_3$
4-Hydroxy-3-ethoxybenzaldehyde
Ethylprotal; ethylvanillin
Bourbonal
Ethovan
NSC 67240
Ethavan
RN: 121-32-4 **MP** (°C)**:** 65
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.019E+00	1.693E+02	25	D407	1 0 2 2 2	

1777. $C_9H_{10}O_3$
Ethyl salicylate
Ethyl *o*-hydroxybenzoate
RN: 118-61-6 **MP** (°C)**:** 1–3
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.032E-02	6.700E+00	37	D009	1 2 1 1 1	0.1N HCl

1778. $C_9H_{10}O_3$
Ethylparaben
4-Hydroxybenzoic acid ethyl ester
Ethyl *p*-hydroxybenzoate
Ethyl 4-hydroxybenzoate
RN: 120-47-8 **MP** (°C)**:** 116
MW: 166.18 **BP** (°C)**:** 297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.750E-03	4.570E-01	15	B355	0 0 0 0 0	
3.370E-03	5.600E-01	20	B355	0 0 0 0 0	
4.910E-03	8.159E-01	20	C006	1 2 1 1 2	
5.329E-03	8.855E-01	25	A059	1 0 1 1 1	
4.090E-03	6.797E-01	25	B355	0 0 0 0 0	
4.510E-03	7.494E-01	25	D081	1 2 2 1 2	
5.300E-03	8.807E-01	25	D339	0 0 0 0 0	
6.310E-03	1.049E+00	25	F322	2 0 1 1 0	EFG
9.628E-03	1.600E+00	25	O027	1 0 1 0 1	
6.379E-03	1.060E+00	25	P013	0 0 0 0 0	
9.500E-03	1.579E+00	27	B129	2 2 2 2 1	
5.200E-03	8.641E-01	27	G078	2 1 0 1 0	EFG
5.400E-03	8.974E-01	27.0	G067	2 0 1 1 1	
6.770E-03	1.125E+00	30	A059	1 0 1 1 2	
8.266E-03	1.374E+00	35	A059	1 0 1 1 2	
7.568E-03	1.258E+00	39.3	G302	2 2 2 2 0	EFG
9.540E-03	1.585E+00	40	A059	1 0 1 1 2	

1779. $C_9H_{10}O_3$
Methyl-4-methoxybenzoate
Methyl anisate
RN: 121-98-2 **MP** (°C)**:** 49
MW: 166.18 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-03	6.431E-01	20	C006	1 0 1 1 2	

1780. $C_9H_{10}O_3$
DL-Tropic acid
DL-Tropasaeure
RN: 529-64-6 **MP** (°C)**:** 118.5
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-01	1.950E+01	20	F300	1 0 0 0 2	

1781. $C_9H_{10}O_4$
3,4-Methoxybenzoic acid
Veratrumsaeure
RN: 93-07-2 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-03	5.000E-01	14	F300	1 0 0 0 0	
3.293E-02	6.000E+00	100	F300	1 0 0 0 0	

1782. $C_9H_{11}BrN_2O_2$
Metobromuron
3-(*p*-Bromophenyl)-1-methoxy-1-methylurea
Patoran
N′-(4-Bromophenyl)-*N*-methoxy-*N*-methylurea
Pattonex
RN: 3060-89-7 **MP** (°C)**:**
MW: 259.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E-03	3.338E-01	20	B179	0 0 0 0 0	
1.274E-03	3.300E-01	20	B200	1 0 0 0 2	
1.274E-03	3.300E-01	20	G036	1 0 0 0 2	
1.274E-03	3.300E-01	20	M061	1 0 0 0 1	
1.274E-03	3.300E-01	20	M161	1 0 0 0 2	
1.157E-03	2.999E-01	ns	B100	0 0 0 0 0	

1783. $C_9H_{11}ClN_2O$

Monuron
N′-(4-Chlorophenyl)-*N,N*-dimethyl-urea
1,1-Dimethyl-3-(*p*-chlorophenyl)urea
RN: 150-68-5 **MP** (°C)**:** 170.5
MW: 198.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-03	2.000E-01	18	F035	1 0 0 0 0	
1.175E-03	2.334E-01	20	B179	0 0 0 0 0	
1.007E-03	2.000E-01	20	E048	1 2 1 1 2	
1.007E-03	2.000E-01	20	F311	1 2 2 2 1	
1.158E-03	2.300E-01	25	A039	1 1 0 0 2	
1.158E-03	2.300E-01	25	B185	0 0 0 0 0	
1.158E-03	2.300E-01	25	B200	1 0 0 0 2	
1.158E-03	2.300E-01	25	G036	1 0 0 0 2	
1.158E-03	2.300E-01	25	G099	1 0 0 1 0	
1.319E-03	2.620E-01	25	H073	2 1 1 2 2	
1.158E-03	2.300E-01	25	M061	1 0 0 0 2	
1.158E-03	2.300E-01	25	M161	1 0 0 0 2	
1.007E-03	2.000E-01	ns	B100	0 0 0 0 0	
1.158E-03	2.300E-01	ns	B160	0 0 0 0 2	
9.000E-04	1.788E-01	ns	F184	0 0 0 0 0	
1.158E-03	2.300E-01	ns	H112	0 0 0 0 2	
1.158E-03	2.300E-01	ns	K007	0 0 0 0 2	
1.158E-03	2.300E-01	ns	N013	0 0 0 0 2	

1784. $C_9H_{11}ClN_2O_2$

Monolinuron
3-(4-Chlorophenyl)-1-methoxy-1-methylurea
Arresin
Afesin
Aresin
RN: 1746-81-2 **MP** (°C)**:** 80
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.692E-03	5.777E-01	20	B179	0 0 0 0 0	
4.333E-03	9.300E-01	20	G036	1 0 0 0 2	
2.702E-03	5.800E-01	20	M061	1 0 0 0 2	
2.702E-03	5.800E-01	22.5	G301	0 0 0 0 0	
3.424E-03	7.350E-01	25	M162	1 1 0 0 2	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.702E-03	5.800E-01	rt	M161	0 0 0 0 2	

1785. $C_9H_{11}ClO$

3-Methyl-5-ethyl-4-chloro-phenol
m-Cresol, 4-chloro-5-ethyl-
RN: 1125-66-2 **MP** (°C)**:**
MW: 170.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	3.754E-01	25	B316	0 0 0 0 0	

1786. $C_9H_{11}Cl_2N_3O_4S_2$

Methylchlothiazide
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-1,1-dioxide
6-Chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
RN: 135-07-9 **MP** (°C)**:**
MW: 360.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.388E-04	5.000E-02	rt	A095	0 0 2 2 0	

1787. $C_9H_{11}Cl_3NO_3PS$

Chlorpyrifos
O,O-Diethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate
DOWCO 179
RN: 2921-88-2 **MP** (°C)**:** 41.5
MW: 350.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.284E-06	4.502E-04	10	B324	0 0 0 0 0	
1.284E-06	4.500E-04	10	B324	0 0 0 0 0	
1.997E-06	7.000E-04	19	B169	2 1 1 1 1	
2.082E-06	7.299E-04	20	B300	2 1 1 1 2	
2.082E-06	7.299E-04	20	B324	0 0 0 0 0	
2.082E-06	7.300E-04	20	B324	0 0 0 0 0	
1.141E-06	4.000E-04	23	B096	1 2 0 0 0	
3.195E-06	1.120E-03	24	F179	2 2 2 2 2	
1.141E-06	4.000E-04	24	K069	2 0 0 1 1	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
5.705E-06	2.000E-03	35	M161	1 0 0 0 0	
1.141E-06	4.000E-04	ns	F071	0 1 2 1 0	
8.557E-07	3.000E-04	ns	K138	0 0 0 0 1	
5.705E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG
3.195E-06	1.120E-03	ns	V414	0 0 0 0 0	
5.705E-06	2.000E-03	ns	Y414	0 0 0 0 0	

1788. $C_9H_{11}Cl_3NO_4P$
Chlorpyrifos oxon
Chlorpyrifos oxygen analog
Dursban oxygen analog
DOWCO 180
3,5,6-Trichloro-2-pyridyl diethyl phosphate
RN: 5598-15-2 **MP** (°C)**:**
MW: 334.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-03	5.200E-01	24	K069	2 0 0 1 1	

1789. $C_9H_{11}FN_2O_3$
2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxopentyl)-
RN: 145303-99-7 **MP** (°C)**:**
MW: 214.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	1.071 E+00	22	B416	2 2 1 2 1	

1790. $C_9H_{11}FN_2O_4$
1-Butyryloxymethyl-5-fluorouracil
Butanoic acid, (5-fluoro-3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)methyl ester
RN: 66542-37-8 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.170E-02	9.600E+00	22	B321	0 0 0 0 0	pH 4.0
4.170E-02	9.600E+00	22	B332	1 1 0 0 1	pH 4.0
4.952E-02	1.140E+01	22	M317	1 1 1 1 1	

1791. $C_9H_{11}FN_2O_4$
1-Isobutyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 2-methylpropyl ester
RN: 71759-45-0 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.000E+00	22	B332	1 1 0 0 1	pH 4.0

1792. $C_9H_{11}FN_2O_4$
1-Butyloxycarbonyl-5-fluorouracil
5-Fluoro-1-(butoxycarbonyl)uracil
RN: 85326-32-5 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.563E-02	5.900E+00	22	B332	1 1 0 0 1	pH 4.0

1793. $C_9H_{11}IN_2O_5$
2′-Deoxy-5-iodouridine
Idoxuridine
(+)-5-Iodo-2′-deoxyuridine
Herplex
RN: 54-42-2 **MP** (°C)**:** 165
MW: 354.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.650E+03	2.001E+06	25	N332	0 0 0 0 0	pH 7.4

1794. $C_9H_{11}N$
1,2,3,4-Tetrahydroquinoline
Kusol
THQ
RN: 635-46-1 **MP** (°C)**:** 15–17
MW: 133.19 **BP** (°C)**:** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	1.404E+00	20.3	L339	2 0 2 2 2	
1.386E-02	1.847E+00	40.0	L339	2 0 2 2 2	
1.774E-02	2.362E+00	59.8	L339	2 0 2 2 2	
2.326E-02	3.098E+00	79.6	L339	2 0 2 2 2	
2.988E-02	3.980E+00	100.4	L339	2 0 2 2 2	

1795. $C_9H_{11}NO$
N-Methylacetanilide
Acetamide, *N*-methyl-*N*-phenyl-
RN: 579-10-2 **MP** (°C)**:** 102
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	2.200E+01	20	B101	0 0 0 0 0	
1.673E-01	2.496E+01	25	B101	0 0 0 0 0	
1.908E-01	2.847E+01	30	B101	0 0 0 0 0	
2.166E-01	3.232E+01	35	B101	0 0 0 0 0	
1.122E-01	1.674E+01	ns	R424	0 0 0 0 0	

1796. $C_9H_{11}NO$
p-Aminopropiophenone
4′-Aminopropiophenone
RN: 70-69-9 **MP** (°C)**:** 140
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-03	3.521E-01	37.5	G002	1 1 1 1 2	pH 6.8

1797. $C_9H_{11}NO$
Propionanilide
Propionsaeure-anilid
Propanilide
RN: 620-71-3 **MP** (°C)**:** 106
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-02	1.800E+00	18	F300	1 0 0 0 1	
1.204E-02	1.797E+00	20	B101	0 0 0 0 0	

1798. $C_9H_{11}NO$
Methyl, [3-(acetylamino)phenyl]-
m-Toluidin-*N*-acetat
m-Toluidine-*N*-acetate
RN: 113321-22-5 **MP** (°C)**:**
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.949E-02	4.400E+00	13	F300	1 0 0 0 1	

1799. $C_9H_{11}NO_2$
Phe
(*S*)-(–)-Phenylalanine
(*S*)-Phenylalanine
2-Amino-3-phenylpropanoic acid
Phenylalanine
RN: 63-91-2 **MP** (°C)**:** 283
MW: 165.19 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-02	9.989E+00	0	D018	2 2 2 1 2	
1.174E-01	1.940E+01	0	F300	1 0 0 0 2	
1.740E-01	2.874E+01	15	D349	2 1 1 2 2	
1.515E-01	2.502E+01	20	B032	1 2 2 1 2	
1.770E-01	2.924E+01	20	D349	2 1 1 2 2	

(*continued*)

1799. $C_9H_{11}NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.637E-01	2.705E+01	25	B032	1 2 2 1 2	
1.740E-01	2.875E+01	25	D041	1 0 0 0 2	
1.800E-01	2.973E+01	25	D349	2 1 1 2 2	
1.816E-01	3.000E+01	25	F300	1 0 0 0 1	
1.649E-01	2.724E+01	25	G092	2 1 1 1 1	
1.649E-01	2.724E+01	25	G315	0 0 0 0 0	
1.625E-01	2.684E+01	25	G433	0 0 0 0 0	
1.589E-01	2.625E+01	25	K031	2 1 2 1 2	
1.200E-01	1.982E+01	25	M097	2 2 2 2 2	
1.494E-01	2.468E+01	25	M374	1 0 2 1 2	
2.100E-01	3.469E+01	25	N001	0 0 0 0 0	EFG
1.720E-01	2.841E+01	25	N012	2 0 2 1 2	
1.574E-01	2.601E+01	25	O316	1 0 1 2 2	
1.575E-01	2.601E+01	25	O316	1 0 1 2 2	
1.689E-01	2.790E+01	25.1	N024	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N025	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N026	0 0 0 0 0	
1.649E-01	2.724E+01	25.1	N027	1 1 2 2 2	
1.717E-01	2.837E+01	27	D036	0 0 0 0 0	
1.683E-01	2.780E+01	27	D036	0 0 0 0 0	
1.834E-01	3.030E+01	28	L081	2 1 2 2 2	
1.790E-01	2.957E+01	29.80	B032	1 2 2 1 2	
2.567E-01	4.240E+01	50	F300	1 0 0 0 2	
3.761E-01	6.212E+01	75	D041	1 0 0 0 2	
3.759E-01	6.210E+01	75	F300	1 0 0 0 2	
4.619E-01	7.630E+01	98	M160	2 1 1 1 0	
5.454E-01	9.010E+01	100	F300	1 0 0 0 2	
9.064E-02	1.497E+01	rt	H431	0 0 0 0 0	

1800. $C_9H_{11}NO_2$

4-(Dimethylamino)benzoic acid

4-Dimethylaminobenzoic acid

RN: 619-84-1 **MP** (°C)**:** 242.5

MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	6.608E-02	ns	C014	0 0 0 1 1	

1801. $C_9H_{11}NO_2$
p-Methoxyacetanilide
p-Acetanisidine
N-(4-Methoxyphenyl)acetamide
N-(4-Methoxyphenyl)acetic acid amide
p-Acetanisidide
Acetamide, *N*-(4-methoxyphenyl)-
RN: 51-66-1 **MP** (°C)**:** 400.3
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.029E-02	1.700E+00	15	F300	1 0 0 0 1	
8.820E-03	1.457E+00	15	M352	1 1 1 1 2	
7.090E-02	1.171E+01	25	D044	0 0 0 0 0	
1.353E-02	2.234E+00	25	M352	1 1 1 1 2	
2.131E-02	3.521E+00	40	M352	1 1 1 1 2	
3.249E-02	5.367E+00	50	M352	1 1 1 1 2	

1802. $C_9H_{11}NO_2$
2-Methyl-4-acetaminophenol
3-Methyl-4-hydroxyacetanilide
3-Methylparacetamol
RN: 16375-90-9 **MP** (°C)**:**
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	4.189E+00	25	D078	1 2 1 1 2	

1803. $C_9H_{11}NO_2$
DL-Phenylalanine
DL-Phenylalanin
RN: 150-30-1 **MP** (°C)**:** 166.5
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.993E-02	9.900E+00	0	F300	1 0 0 0 1	
9.080E-02	1.500E+01	21	F300	1 0 0 0 1	
9.008E-02	1.488E+01	21	P045	1 0 2 1 2	
8.464E-02	1.398E+01	25	D018	2 2 2 1 2	
8.476E-02	1.400E+01	25	D041	1 0 0 0 2	
1.304E-01	2.154E+01	50	D018	2 2 2 1 2	
1.295E-01	2.140E+01	50	F300	1 0 0 0 2	
2.158E-01	3.564E+01	75	D018	2 2 2 1 2	
2.164E-01	3.575E+01	75	D041	1 0 0 0 2	
2.167E-01	3.580E+01	75	F300	1 0 0 0 2	
3.898E-01	6.440E+01	100	F300	1 0 0 0 2	

1804. $C_9H_{11}NO_2$
m-Tolyl methylcarbamate
3-Tolyl methylcarbamate
RN: 1129-41-5 **MP** (°C)**:** 76.5
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.574E-02	2.600E+00	30	M161	1 0 0 0 1	

1805. $C_9H_{11}NO_2$
D-Phenylalanine
D-α-Aminohydrocinnamic acid
D-α-Amino-β-phenylpropionic acid
D-β-Phenyl-α-aminopropionic acid
D-PHE
RN: 673-06-3 **MP** (°C)**:** 273
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.763E-01	2.913E+01	25	D041	1 0 0 0 0	

1806. $C_9H_{11}NO_2$
Ethyl *p*-aminobenzoate
4-Aminobenzoic acid ethyl ester
Ethyl *p*-aminobenzoic acid
Benzocaine
RN: 94-09-7 **MP** (°C)**:** 89.0
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.308E-03	7.117E-01	15	M352	1 1 1 1 2	
1.513E-02	2.500E+00	20	F300	1 0 0 0 1	
5.800E-03	9.581E-01	25	A418	0 0 0 0 0	
4.840E-03	7.995E-01	25	H008	0 0 0 0 0	
6.493E-03	1.073E+00	25	M352	1 1 1 1 2	
6.216E-03	1.027E+00	25	P303	0 0 0 0 0	
6.980E-03	1.153E+00	30	A418	0 0 0 0 0	
7.930E-03	1.310E+00	30	B071	1 2 1 1 2	
5.150E-03	8.507E-01	30	H018	0 0 0 0 0	
7.500E-03	1.239E+00	30	J018	1 2 0 1 1	0.05N NaOH
7.000E-03	1.156E+00	30	L069	1 0 1 1 0	EFG
7.680E-03	1.269E+00	30	R003	0 0 0 0 0	
8.156E-03	1.347E+00	33	P303	0 0 0 0 0	
8.750E-03	1.445E+00	35	A418	0 0 0 0 0	
1.020E-02	1.685E+00	37	F006	1 1 2 2 2	
1.024E-02	1.692E+00	40	A418	0 0 0 0 0	
1.164E-02	1.924E+00	40	M352	1 1 1 1 2	

(*continued*)

1806. $C_9H_{11}NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-02	1.704E+00	40	P303	0 0 0 0 0	
1.701E-02	2.810E+00	50	M352	1 1 1 1 2	
>3.03E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.810E-03	7.946E-01	ns	M066	0 0 0 0 2	
4.810E-03	7.946E-01	rt	B016	0 0 1 1 2	pH 7.4
5.135E-03	8.483E-01	rt	I404	0 0 0 0 0	Average

1807. $C_9H_{11}NO_3$

L-Tyrosine
3-(4-Hydroxyphenyl)-L-alanine
Tyrosine
(*S*)-(–)-Tyrosine
p-Tyrosine
L-Tyrosin

RN: 60-18-4 **MP** (°C)**:** 342dec
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.241E-03	2.249E-01	0	D018	2 2 2 1 2	
1.104E-03	2.000E-01	0	F300	1 0 0 0 0	
2.042E-03	3.700E-01	20	B032	1 2 2 1 2	
2.495E-03	4.520E-01	21	P045	1 0 2 1 2	
2.285E-03	4.140E-01	22	A045	2 0 2 2 2	
2.800E-03	5.073E-01	24.99	C404	2 1 2 2 1	
7.800E-02	1.413E+01	25	C405	2 1 2 2 2	intrinsic zwit
2.642E-03	4.788E-01	25	D018	2 2 2 1 2	
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
2.759E-03	5.000E-01	25	F300	1 0 0 0 0	
2.444E-03	4.428E-01	25	G433	0 0 0 0 0	
2.620E-03	4.747E-01	25	H097	2 2 2 2 2	
2.622E-03	4.750E-01	25.1	N024	0 0 0 0 0	
2.495E-03	4.520E-01	25.1	N025	0 0 0 0 0	
2.489E-03	4.510E-01	25.1	N026	0 0 0 0 0	
2.488E-03	4.508E-01	25.1	N027	1 1 2 2 2	
2.753E-03	4.988E-01	27	D036	0 0 0 0 0	
2.677E-03	4.850E-01	27	D036	0 0 0 0 0	
3.195E-03	5.790E-01	28	L081	2 1 2 2 2	
3.800E-03	6.885E-01	34.99	C404	2 1 2 2 1	
5.050E-03	9.150E-01	44.99	C404	2 1 2 2 1	
6.064E-03	1.099E+00	50	D018	2 2 2 1 2	
6.071E-03	1.100E+00	50	F300	1 0 0 0 1	
1.309E-02	2.372E+00	75	D018	2 2 2 1 2	
1.343E-02	2.434E+00	75	D041	1 0 0 0 2	
1.325E-02	2.400E+00	75	F300	1 0 0 0 1	
3.091E-02	5.600E+00	100	F300	1 0 0 0 1	

1808. $C_9H_{11}NO_3$
D-Tyrosine
3-(4-Hydroxyphenyl)-D-alanine
RN: 556-02-5 **MP** (°C)**:** >300
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
5.789E-03	1.049E+00	50	D041	1 0 0 0 2	

1809. $C_9H_{11}NO_3$
DL-Tyrosine
DL-Tyrosin
3-(4-Hydroxyphenyl)-DL-alanine
DL-2-Amino-3-(4-hydroxyphenyl)-propanoic acid
RN: 556-03-6 **MP** (°C)**:** 325
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.519E-04	1.000E-01	0	F300	1 0 0 0 0	
2.208E-03	4.000E-01	20	F300	1 0 0 0 0	
1.936E-03	3.509E-01	25	D041	1 0 0 0 2	
4.610E-03	8.353E-01	50	D041	1 0 0 0 2	
4.415E-03	8.000E-01	50	F300	1 0 0 0 0	
3.753E-02	6.800E+00	100	F300	1 0 0 0 1	

1810. $C_9H_{11}NO_4$
Dopa
DL-3-(3,4-Dihydroxyphenyl)alanine
DL-Dopa
RN: 63-84-3 **MP** (°C)**:** >270
MW: 197.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	4.975E+00	20	D041	1 0 0 0 0	
1.237E-01	2.439E+01	100	D041	1 0 0 0 1	

1811. $C_9H_{11}NO_4$
Levodopa
L-3,4-Dihydroxyphenylalanin
RN: 59-92-7 **MP** (°C)**:** 277
MW: 197.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	5.000E+00	20	F300	1 0 0 0 0	
1.917E-02	3.780E+00	25	H015	1 0 0 0 2	

(*continued*)

1811. $C_9H_{11}NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.927E-02	3.800E+00	25.1	N025	0 0 0 0 0	
1.268E-01	2.500E+01	100	F300	1 0 0 0 1	
5.071E-03	1.000E+00	ns	K444	0 0 0 0 0	

1812. $C_9H_{11}NS_2Hg$

Phenylmercury dimethyldithiocarbamate
Chipman merbam
Merfenl 51
Phelam DP

RN: 32407-99-1 **MP** (°C)**:** 175
MW: 397.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.508E-05	6.000E-03	20	M161	1 0 0 0 0	

1813. $C_9H_{11}N_3O$

Biacetyl mono(2-pyridyl)-hydrazone
BPH
Biacetyl mono(2-pyridyl)hydrazone

RN: 74158-10-4 **MP** (°C)**:** 95
MW: 177.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.643E-04	9.999E-02	ns	R080	0 0 0 0 0	

1814. $C_9H_{11}N_3O_2S_2$

Sulfathiazoline
Benzenesulfonamide, 4-amino-*N*-(4,5-dihydro-2-thiazolyl)-

RN: 32365-02-9 **MP** (°C)**:**
MW: 257.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-04	1.490E-01	20	F073	1 2 2 2 2	

1815. $C_9H_{11}N_3O_4$

Orotic acid morpholine

RN: **MP** (°C)**:** 289–291
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-01	9.909E+01	–4	N018	0 0 0 0 0	
6.500E-01	1.464E+02	16	N018	0 0 0 0 0	
7.450E-01	1.678E+02	25	N018	0 0 0 0 0	

1816. $C_9H_{11}O_4P$
2-Carboxyethylphenylphosphinic acid
CEPPA
RN: **MP** (°C)**:**
MW: 214.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-02	2.076E+01	25.1	W412	0 0 0 0 0	
1.947E-01	4.171E+01	35.51	W412	0 0 0 0 0	
3.450E-01	7.389E+01	44.92	W412	0 0 0 0 0	
6.388E-01	1.368E+02	54.02	W412	0 0 0 0 0	
1.068E+00	2.287E+02	64.60	W412	0 0 0 0 0	
1.341E+00	2.873E+02	69.60	W412	0 0 0 0 0	
1.536E+00	3.290E+02	71.91	W412	0 0 0 0 0	
1.883E+00	4.034E+02	76.32	W412	0 0 0 0 0	

1817. C_9H_{12}
1,2,3-Trimethylbenzene
Hemimellitene
Hemellitol
RN: 526-73-8 **MP** (°C)**:** –25
MW: 120.20 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.450E-04	6.551E-02	25	M342	1 0 1 1 2	
6.256E-04	7.520E-02	25	S005	2 2 2 2 2	
6.256E-04	7.520E-02	25	S191	1 2 2 2 2	
6.256E-04	7.520E-02	25	S358	2 2 2 2 2	

1818. C_9H_{12}
1-Ethyl-2-methylbenzene
2-Ethyltoluene
o-Ethyltoluene
1-Methyl-2-ethylbenzene
RN: 611-14-3 **MP** (°C)**:** –80.8
MW: 120.20 **BP** (°C)**:** 165.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.210E-04	7.464E-02	25	M342	1 0 1 1 2	
7.742E-04	9.305E-02	ns	H123	0 0 0 0 0	

1819. C_9H_{12}
1,8-Nonadiyne
RN: 2396-65-8 **MP** (°C)**:** –21
MW: 120.20 **BP** (°C)**:** 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-03	1.250E-01	25	M001	2 1 2 2 2	

1820. C_9H_{12}
Cumene
Isopropylbenzene
Cumol
2-Phenylpropane
RN: 98-82-8 **MP** (°C)**:** –96
MW: 120.20 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.694E-04	8.046E-02	24.94	G034	1 2 2 2 2	
6.073E-04	7.300E-02	25	A002	1 2 1 1 1	
4.018E-04	4.830E-02	25	K119	1 0 0 0 2	
4.160E-04	5.000E-02	25	M001	2 1 2 2 2	
4.409E-04	5.300E-02	25	M002	2 2 1 2 1	
4.160E-04	5.000E-02	25	M130	1 0 0 0 1	
4.018E-04	4.830E-02	25	P051	2 1 1 2 2	
5.433E-04	6.530E-02	25	S005	2 2 2 2 2	
5.433E-04	6.530E-02	25	S191	1 2 2 2 2	
5.433E-04	6.530E-02	25	S358	2 1 2 2 2	
4.018E-04	4.830E-02	25.00	P007	2 1 2 2 2	
6.897E-04	8.290E-02	29.94	G034	1 2 2 2 2	
7.124E-04	8.563E-02	34.94	G034	1 2 2 2 2	
7.469E-04	8.978E-02	39.94	G034	1 2 2 2 2	
7.867E-04	9.456E-02	44.94	G034	1 2 2 2 2	
8.353E-04	1.004E-01	49.94	G034	1 2 2 2 2	
8.894E-04	1.069E-01	54.94	G034	1 2 2 2 2	
9.566E-04	1.150E-01	59.94	G034	1 2 2 2 2	
1.035E-03	1.243E-01	65.14	G034	1 2 2 2 2	
1.128E-03	1.355E-01	70.34	G034	1 2 2 2 2	
1.226E-03	1.473E-01	75.04	G034	1 2 2 2 2	
1.345E-03	1.617E-01	80.24	G034	1 2 2 2 2	
4.160E-04	5.000E-02	ns	H123	0 0 0 0 0	
4.160E-04	5.000E-02	ns	M344	0 0 0 0 1	

1821. C_9H_{12}
n-Propylbenzene
1-Phenylpropane
Propylbenzene
Isocomene
RN: 103-65-1 **MP** (°C)**:** –99.2
MW: 120.20 **BP** (°C)**:** 159.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-04	5.373E-02	10	O312	2 2 0 2 2	
5.000E-04	6.010E-02	15	F001	1 0 1 2 0	
4.350E-04	5.229E-02	15	O312	2 2 0 2 2	
4.520E-04	5.433E-02	20	O312	2 2 0 2 2	
4.576E-04	5.500E-02	25	A002	1 2 1 1 1	
1.000E-03	1.202E-01	25	K001	1 0 2 1 2	

(*continued*)

1821. C_9H_{12} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.340E-04	5.217E-02	25	M342	1 0 1 1 2	
4.430E-04	5.325E-02	25	O312	2 2 0 2 2	
8.319E-04	9.999E-02	25	S012	2 0 2 2 1	
4.150E-04	4.988E-02	25	S359	2 1 2 2 2	
3.920E-04	4.712E-02	25	T067	2 1 2 1 2	
4.340E-04	5.217E-02	25	W300	2 2 2 2 2	
4.370E-04	5.253E-02	30	O312	2 2 0 2 2	
4.710E-04	5.661E-02	35	O312	2 2 0 2 2	
5.320E-04	6.394E-02	40	O312	2 2 0 2 2	
5.540E-04	6.659E-02	45	O312	2 2 0 2 2	
1.098E-03	1.320E-01	85.8	G035	1 0 0 0 2	
1.381E-03	1.660E-01	114.5	G035	1 0 0 0 2	
2.670E-03	3.209E-01	140.5	G035	1 0 0 0 2	
7.232E-03	8.692E-01	188.0	G035	1 0 0 0 1	
2.033E-02	2.444E+00	222.0	G035	1 0 0 0 2	
4.576E-04	5.500E-02	ns	H123	0 0 0 0 0	
2.700E-02	3.245E+00	ns	H307	0 0 0 0 0	
4.576E-04	5.500E-02	ns	M344	0 0 0 0 1	

1822. C_9H_{12}
1,2,4-Trimethylbenzene
Pseudocumene
RN: 95-63-6 **MP** (°C)**:** –44
MW: 120.20 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.318E-04	5.190E-02	25	K119	1 0 0 0 2	
4.742E-04	5.700E-02	25	M001	2 1 2 2 2	
4.318E-04	5.190E-02	25	P051	2 1 1 2 2	
4.909E-04	5.900E-02	25	S005	2 2 2 2 2	
4.909E-04	5.900E-02	25	S191	1 2 2 2 2	
4.909E-04	5.900E-02	25	S358	2 1 2 2 2	
4.318E-04	5.190E-02	25.00	P007	2 1 2 2 2	
4.742E-04	5.700E-02	ns	M344	0 0 0 0 1	

1823. C_9H_{12}
p-Ethyltoluene
4-Ethyltoluene
1-Ethyl-4-methylbenzene
RN: 622-96-8 **MP** (°C)**:** –62
MW: 120.20 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.891E-04	9.485E-02	ns	H123	0 0 0 0 0	

1824. C_9H_{12}

Mesitylene
1,3,5-Trimethylbenzene
Mesitelene

RN: 108-67-8 **MP** (°C)**:** –44.8
MW: 120.20 **BP** (°C)**:** 164.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.794E-04	4.560E-02	15	S203	1 1 2 1 2	
3.111E-04	3.740E-02	20	M337	2 1 2 2 2	
8.070E-04	9.700E-02	25	A002	1 2 1 1 1	
4.010E-04	4.820E-02	25	S005	2 2 2 2 2	
4.010E-04	4.820E-02	25	S191	1 2 2 2 2	
4.118E-04	4.950E-02	25	S203	1 1 2 1 2	
4.010E-04	4.820E-02	25	S358	2 1 2 2 2	
3.280E-04	3.942E-02	25.04	V013	2 2 2 2 2	
5.322E-04	6.397E-02	29.99	C350	0 0 0 0 0	
4.509E-04	5.420E-02	35	S203	1 1 2 1 2	
5.555E-04	6.677E-02	39.99	C350	0 0 0 0 0	
4.701E-04	5.650E-02	45	S203	1 1 2 1 2	
6.166E-04	7.412E-02	49.99	C350	0 0 0 0 0	
7.555E-04	9.081E-02	59.99	C350	0 0 0 0 0	
9.221E-04	1.108E-01	69.99	C350	0 0 0 0 0	
1.161E-03	1.395E-01	79.99	C350	0 0 0 0 0	
1.361E-03	1.636E-01	89.99	C350	0 0 0 0 0	
1.616E-03	1.943E-01	99.99	C350	0 0 0 0 0	

1825. $C_9H_{12}ClN_5O$

Moxonidine

RN: 75438-57-2 **MP** (°C)**:**
MW: 241.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-03	8.003E-01	ns	R426	0 0 0 0 0	

1826. $C_9H_{12}ClO_2PS_3$

Carbophenothion-methyl
S-p-Chlorophenylthiomethyl *O,O*-dimethyl phosphorodithioate

RN: 953-17-3 **MP** (°C)**:**
MW: 314.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.669E-06	1.470E-03	10	B324	0 0 0 0 0	
4.670E-06	1.470E-03	10	B324	0 0 0 0 0	
5.178E-06	1.630E-03	20	B300	2 1 1 1 2	
5.083E-06	1.600E-03	20	B324	0 0 0 0 0	
5.082E-06	1.600E-03	20	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
3.176E-06	1.000E-03	rt	M161	0 0 0 0 0	

1827. $C_9H_{12}ClO_4P$
Heptenophos
7-Chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl phosphate
Ragadan
Hostaquick
RN: 23560-59-0 **MP** (°C)**:**
MW: 250.62 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.975E-03	2.500E+00	23	M161	1 0 0 0 1	

1828. $C_9H_{12}Cl_2N_4$
2,4-Dichloro-6-cyclohexylamino-1,3,5-triazine
2,4-Dichloro-6-(cyclohexylamino)triazine
1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-cyclohexyl-
RN: 27282-86-6 **MP** (°C)**:**
MW: 247.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.046E-04	1.000E-01	ns	B160	0 0 0 0 2	

1829. $C_9H_{12}FN_3O_3$
1-Butylcarbamoyl-5-fluorouracil
N-Butyl-5-fluoro-2,4-dioxo-pyrimidinecarboxamide
RN: 64098-82-4 **MP** (°C)**:** 136
MW: 229.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.577E-03	8.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.577E-03	8.200E-01	22	B388	0 0 0 0 0	

1830. $C_9H_{12}NO_5PS$
Fenitrothion
Dimethyl *O*-(4-nitro-*m*-tolyl) phosphorothioate
Nuvanol
Novathion
Dybar
Metathionine
RN: 122-14-5 **MP** (°C)**:** 3.4
MW: 277.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.089E-05	2.520E-02	20	B169	2 0 1 1 2	
1.396E-04	3.870E-02	22	K137	1 1 2 1 0	*sic*
1.082E-04	3.000E-02	ns	F071	0 1 2 1 1	
1.082E-04	3.000E-02	ns	M061	0 0 0 0 1	
1.082E-04	3.000E-02	ns	M110	0 0 0 0 0	EFG

1831. $C_9H_{12}NO_5PS$

O-Methyl *O*-ethyl *O*-4-nitrophenyl thiophosphate
Ethylmethylthiophos
Methylethylthiophos
Methylethylthiofos

RN: 2591-57-3 **MP** (°C)**:**
MW: 277.24 **BP** (°C)**:** 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-04	4.000E-02	ns	M061	0 0 0 0 1	

1832. $C_9H_{12}N_2O$

Fenuron
3-Phenyl-1,1-dimethylurea
N,N-Dimethyl-*N*-phenylurea
Beet-Klean

RN: 101-42-8 **MP** (°C)**:** 133–134
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-02	3.849E+00	20	B179	0 0 0 0 0	
2.245E-02	3.686E+00	20	E048	1 2 1 1 2	
2.253E-02	3.700E+00	20	F311	1 2 2 2 1	
1.766E-02	2.900E+00	24	B185	0 0 0 0 0	
1.761E-02	2.892E+00	24	M061	1 0 0 0 1	
1.462E-02	2.400E+00	25	A039	1 1 0 0 2	
2.345E-02	3.850E+00	25	B200	1 0 0 0 0	
2.345E-02	3.850E+00	25	G036	1 0 0 0 2	
1.462E-02	2.400E+00	25	G099	1 0 0 1 0	
2.452E-02	4.027E+00	25	H073	2 1 1 2 2	
2.345E-02	3.850E+00	25	M161	1 0 0 0 2	
2.426E-02	3.984E+00	ns	B100	0 0 0 0 0	
1.462E-02	2.400E+00	ns	B160	0 0 0 0 2	
2.345E-02	3.850E+00	ns	B185	0 0 0 0 0	
1.761E-02	2.892E+00	ns	N013	0 0 0 0 1	

1833. $C_9H_{12}N_2O_2$

Dulcin
(4-Ethoxyphenyl)urea
4-Aethoxy-phenylharnstoff

RN: 150-69-6 **MP** (°C)**:** 173
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.714E-03	1.210E+00	21	F300	1 0 0 0 2	
7.214E-03	1.300E+00	45	F300	1 0 0 0 1	
1.110E-01	2.000E+01	100	F300	1 0 0 0 0	
6.928E-03	1.248E+00	c	I314	0 0 0 0 0	
1.088E-01	1.961E+01	h	I314	0 0 0 0 0	

1834. $C_9H_{12}N_2O_2S$
3-Thio-2,4-diazaspiro[5.5]undecane-1,3,5-trione
2,4-Diazaspiro[5.5]undecane-1,5-dione, 3-thioxo-
2,4-Diazaspiro[5.5]undecane-1,3,5-trione, 3-thio
RN: 52-45-9 **MP** (°C)**:**
MW: 212.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	7.323E-02	25	P350	0 0 0 0 0	intrinsic

1835. $C_9H_{12}N_2O_3$
5-Allyl-5-ethylbarbituric acid
Barbituric acid, 5-allyl-5-ethyl
5-Ethyl-5-allylbarbituric acid
Dormitiv
5-Ethyl-5-allylbarbiturate
RN: 2373-84-4 **MP** (°C)**:**
MW: 196.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	4.774E+00	25	P350	0 0 0 0 0	intrinsic

1836. $C_9H_{12}N_2O_3$
2,4-Diazaspiro[5.5]undecane-1,3,5-trione
Spiro[barbituric acid-5,1′-cyclohexane]
Cyclohexane-spirobarbiturate
RN: 52-44-8 **MP** (°C)**:**
MW: 196.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	1.707E-01	25	P350	0 0 0 0 0	intrinsic

1837. $C_9H_{12}N_2O_5$
Deoxyuridine
RN: 951-78-0 **MP** (°C)**:** 168
MW: 228.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	4.685E+02	25.31	T420	0 0 0 0 0	

1838. $C_9H_{12}N_2O_6$
Uridine
RN: 58-96-8 **MP** (°C)**:** 166.5
MW: 244.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.40E+00	~8.30E+02	21.99	T418	0 0 0 0 0	
~3.20E+00	~7.81E+02	22.99	T418	0 0 0 0 0	

1839. $C_9H_{12}N_4O_2$
7-Ethyl theophylline
7-Ethyl-1,3-dimethylxanthine
1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-1,3-dimethyl-
RN: 23043-88-1 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-01	3.665E+01	30	B042	1 2 1 1 2	
1.760E-01	3.665E+01	30	G021	1 0 0 0 2	

1840. $C_9H_{12}N_4O_2$
1-Ethyl theobromine
1-Ethyl-3,7-dimethylxanthine
1H-Purine-2,6-dione, 1-ethyl-3,7-dihydro-3,7-dimethyl-
RN: 39832-36-5 **MP** (°C)**:** 156
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-01	3.977E+01	30	B042	1 2 1 1 2	
1.910E-01	3.977E+01	30	G021	1 0 0 0 2	

1841. $C_9H_{12}N_4O_2$
1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-ethoxyethoxy)-
1-Ethoxyethyl-4-allopurinyl ether
RN: 52717-51-8 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.173E-03	1.910E+00	ns	H067	0 0 0 0 0	

1842. $C_9H_{12}N_4O_2$
8-Methyl caffeine
1,3,7,8-Tetramethylxanthine
RN: 832-66-6 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-02	2.175E+00	20	J009	1 0 2 2 2	

1843. $C_9H_{12}N_4O_3$
7-β-Hydroxyethyltheophylline
1H-Purine-2,6-dione, 3,7-Dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-
Dilaphyllin
Etofylline
Corophyllin-*N*
RN: 519-37-9 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	3.226E+01	ns	J025	0 0 0 0 1	

1844. $C_9H_{12}N_4O_3$
8-Methoxycaffeine
1H-Purine-2,6-dione, 3,7-dihydro-8-methoxy-1,3,7-trimethyl-
RN: 569-34-6 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-02	2.556E+00	25	K008	1 1 0 1 0	EFG
1.115E-04	2.500E-02	rt	N015	0 0 2 2 1	

1845. $C_9H_{12}N_4O_3$
1,3,7,9-Tetramethyluric acid
1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7,9-tetramethyl-
Temorine
Temurin
Ba 2750
RN: 2309-49-1 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.472E-04	3.300E-02	rt	N015	0 0 2 2 1	

1846. $C_9H_{12}N_4O_3S$
*N*4-Acetylsulfanilylguanidine
Acetamide, *N*-[4-[[(aminoiminomethyl)amino]sulfonyl]phenyl]-
p-(Guanidinosulfonyl)acetanilide
Sulgin ASG
RN: 19077-97-5 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-03	3.998E-01	37.50	M142	1 2 0 0 1	
5.766E-02	1.478E+01	h	M142	0 0 0 0 1	

1847. $C_9H_{12}O$
2,3,5-Trimethyl-phenol
Isopseudocumenol
1-Hydroxy-2,3,5-trimethylbenzene
RN: 697-82-5 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	7.627E-01	25	B316	0 0 0 0 0	

1848. $C_9H_{12}O$
4-Propylphenol
4-Propyphenol
p-*n*-Propylphenol
RN: 645-56-7 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-02	1.427E+00	25	L022	1 0 0 0 0	

1849. $C_9H_{12}O$
2-Propylphenol
2-*n*-Propylphenol
2-Propyphenol
RN: 644-35-9 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.222E-02	1.664E+00	25	L022	1 0 0 0 0	

1850. $C_9H_{12}O$
3-Methyl-5-ethyl-phenol
Phenol, 3-ethyl-5-methyl-
m-Cresol, 5-ethyl-
RN: 698-71-5 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	2.315E+00	25	B316	0 0 0 0 0	

1851. $C_9H_{12}O$
4-Ethyl-3-methylphenol
3-Methyl-4-ethylphenol
4-Ethyl-*m*-cresol
RN: 1123-94-0 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-03	9.990E-01	25	L020	1 0 0 0 0	

1852. $C_9H_{12}O$
2,4,6-Trimethylphenol
2-Hydroxymesitylene
1-Hydroxy-2,4,6-trimethylbenzene
Mesityl alcohol
Hydroxymesitylene
RN: 527-60-6 **MP** (°C)**:** 72
MW: 136.20 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.008E+00	25	B316	0 0 0 0 0	
4.892E-03	6.662E-01	25	L020	1 0 0 0 0	

1853. $C_9H_{12}O_2$
o-Propoxyphenol
2-Propoxyphenol
RN: 6280-96-2 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.359E+00	24.99	B353	0 0 0 0 0	

1854. $C_9H_{12}O_2$
Cumene hydroperoxide
CHP
RN: 80-15-9 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.140E-02	1.391E+01	25	K051	1 2 2 1 2	

1855. $C_9H_{12}O_2$
3-Propoxyphenol
m-Propoxy phenol
Phenol, 3-propoxy-
RN: 16533-50-9 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	3.942E+00	30	B315	0 0 0 0 0	

1856. $C_9H_{12}O_2$
1-*O*-Benzylethanediol
Benzylcellosolve
Benzyl cellosolve
RN: 622-08-2 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.618E-02	3.984E+00	20	D052	1 1 0 0 0	
2.813E-02	4.282E+00	23	M062	1 0 0 0 1	

1857. $C_9H_{13}BrN_2O_2$
5-Bromo-3-*tert*-butyl-6-methyluracil
Compound 733
RN: 7286-76-2 **MP** (°C)**:** 188
MW: 261.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.570E-03	4.100E-01	25	M061	1 0 0 0 0	
3.121E-03	8.150E-01	ns	B185	0 0 0 0 0	

1858. $C_9H_{13}BrN_2O_2$
Bromacil
5-Bromo-6-methyl-3,5-butyluracil
RN: 314-40-9 **MP** (°C)**:** 158.3
MW: 261.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	7.100E-01	25	B200	1 0 0 0 2	
3.119E-03	8.143E-01	25	B200	1 0 0 0 2	
3.121E-03	8.150E-01	25	M061	1 0 0 0 2	
3.121E-03	8.150E-01	25	M161	1 0 0 0 2	
3.061E-03	7.994E-01	ns	B100	0 0 0 0 0	

1859. $C_9H_{13}ClN_2O_2$
Terbacil
3-*tert*-Butyl-5-chloro-6-methyluracil
5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione
Sinbar 80W
Geonter
DPX-D732
RN: 5902-51-2 **MP** (°C)**:** 176.0
MW: 216.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.277E-03	7.100E-01	25	M061	1 0 0 0 2	
3.277E-03	7.100E-01	25	M161	1 0 0 0 2	
3.277E-03	7.100E-01	25	P307	1 0 0 0 1	
3.228E-03	6.995E-01	ns	B100	0 0 0 0 0	

1860. $C_9H_{13}ClN_6$
Cyanazine
Bladex
2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile
Fortrol
Payze
SD 45418
RN: 21725-46-2 **MP** (°C)**:** 166.5
MW: 240.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.647E-04	1.600E-01	23	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	M061	1 0 0 0 2	
7.104E-04	1.710E-01	25	M161	1 0 0 0 2	
6.647E-04	1.600E-01	25	S309	1 0 0 0 2	
8.309E-04	2.000E-01	ns	M110	0 0 0 0 0	EFG

1861. $C_9H_{13}N$
2,4,5-Trimethylaniline
2,4,5-Trimethylanilin
RN: 137-17-7 **MP** (°C)**:**
MW: 135.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.875E-03	1.200E+00	19.40	F300	1 0 0 0 1	
1.109E-02	1.500E+00	28.70	F300	1 0 0 0 1	

1862. $C_9H_{13}NO_3$
Adrenaline
Adrenalin
Epinephrine
L-1-(3,4-Dihydroxyphenyl)-2-methylaminoethanol
Primatene
Epipen
RN: 51-43-4 **MP** (°C)**:**
MW: 183.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.825E-04	1.800E-01	20	F300	1 0 0 0 1	

1863. $C_9H_{13}N_3O_3$
Orotic acid *n*-butylamide
Orotamide, *N*-butyl-
RN: 13156-38-2 **MP** (°C)**:** 276–277
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.204E+01	–4	N018	0 0 0 0 0	
9.600E-02	2.028E+01	16	N018	0 0 0 0 0	
1.180E-01	2.492E+01	25	N018	0 0 0 0 0	

1864. $C_9H_{13}N_3O_3$
Zalcitabine
2′,3′-Dideoxycytidine
Dideoxycytidine
CCRIS 692
Hivid
DDCYD
RN: 7481-89-2 **MP** (°C)**:** 210–214
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.360E-01	7.098E+01	ns	S469	0 0 0 0 0	

1865. $C_9H_{13}N_3O_3$
Orotic acid diethylamine
Orotamide, *N,N*-diethyl-
RN: 883-81-8 **MP** (°C)**:** 192–194
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E+00	6.208E+02	25	N018	0 0 0 0 0	

1866. $C_9H_{13}N_3O_4$
Orotic acid isobutanolamine
RN: **MP** (°C)**:** 247–249
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	9.543E+01	–4	N018	0 0 0 0 0	
7.060E-01	1.604E+02	16	N018	0 0 0 0 0	
8.410E-01	1.911E+02	25	N018	0 0 0 0 0	

1867. $C_9H_{13}N_3O_4$
Cytosine deoxyriboside
RN: 951-77-9 **MP** (°C)**:**
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E+00	6.317E+02	25.23	T420	0 0 0 0 0	

1868. $C_9H_{13}N_3O_5$
Cytidine
RN: 65-46-3 **MP** (°C)**:** > 215
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.70E-01	~2.36E+02	21.99	T418	0 0 0 0 0	
~8.00E-01	~1.95E+02	22.99	T418	0 0 0 0 0	

1869. $C_9H_{13}N_3O_5$
Orotic acid 2-amide-2-methyl-1,3-propanediol
RN: **MP** (°C)**:** 214–215
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-01	8.391E+01	–4	N018	0 0 0 0 0	
5.860E-01	1.425E+02	16	N018	0 0 0 0 0	
6.970E-01	1.695E+02	25	N018	0 0 0 0 0	

1870. $C_9H_{13}N_5O_4$
Ganciclovir
2-Amino-1,9-dihydro-9-((2-hydroxy-1-(hydroxymethyl)ethoxy)methyl)-6H-purin-6-one
DHPG
RN: 82410-32-0 **MP** (°C)**:** 250
MW: 255.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	3.600E+00	25	B360	0 0 0 0 0	
1.230E-02	3.139E+00	25	Z407	0 0 0 0 0	

1871. $C_9H_{13}O_2P$
Mesitylene phosphinous acid
Phosphinic acid, (2,4,6-trimethylphenyl)-
RN: 6781-97-1 **MP** (°C)**:** 147.0
MW: 184.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.882E+00	1	C061	2 2 2 1 2	
1.619E-02	2.981E+00	25	C061	2 2 2 1 2	
1.754E-02	3.230E+00	35	C061	2 2 2 1 2	
2.082E-02	3.835E+00	45	C061	2 2 2 1 2	
2.836E-02	5.223E+00	65	C061	2 2 2 1 2	
3.774E-02	6.951E+00	85	C061	2 2 2 1 2	

1872. $C_9H_{13}O_6PS$
Endothion
O,O-Dimethyl *S*-(5-methoxypyronyl-2-methyl) thiophosphate
RN: 2778-04-3 **MP** (°C)**:** 90.5
MW: 280.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.141E+00	6.000E+02	ns	M061	0 0 0 0 2	
5.353E+00	1.500E+03	ns	M161	0 0 0 0 1	

1873. $C_9H_{14}ClN_5$
Cyprozine
2-Chloro-4-cyclopropylamino-6-isopropylamino-1,3,5-triazine
RN: 22936-86-3 **MP** (°C)**:** 167
MW: 227.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.030E-05	6.900E-03	25	B200	1 0 0 0 1	
8.582E-04	1.954E-01	40	B200	1 0 0 0 2	

1874. $C_9H_{14}N_2O_3$
5-Ethyl-5-*n*-propylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-propyl-
5-Ethyl-5-propylbarbiturate
RN: 33376-25-9 **MP** (°C)**:** 146.5
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.872E-02	5.694E+00	25	B065	1 2 1 1 1	
3.610E-02	7.156E+00	25	M310	2 2 2 2 2	

1875. $C_9H_{14}N_2O_3$
Metharbital
5,5′-Diethyl-1-methylbarbituric acid
RN: 50-11-3 **MP** (°C)**:** 155
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-02	2.000E+00	25	B011	2 0 0 1 0	
9.980E-03	1.978E+00	25	B065	1 1 1 1 1	
1.150E-02	2.280E+00	25	G003	1 1 1 1 2	pH 4.7
6.054E-03	1.200E+00	25	P061	0 0 0 0 0	
4.979E-03	9.870E-01	rt	M161	0 0 0 0 2	

1876. $C_9H_{14}N_2O_3$
Probarbital
5-Ethyl-5-isopropylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylethyl)
RN: 76-76-6 **MP** (°C)**:** 197.5
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.104E-03	1.210E+00	25	B065	1 1 1 1 1	
7.111E-03	1.410E+00	25	P350	0 0 0 0 0	intrinsic
1.210E-01	2.399E+01	40	N008	1 0 1 1 2	*sic*

1877. $C_9H_{14}N_6$
6-Amino-4-(diallylamino)-1,2-dihydro-1-hydroxy-2-imino-*s*-triazine
RN: **MP** (°C)**:**
MW: 206.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-01	3.010E+01	37	H004	0 0 0 0 0	

1878. $C_9H_{14}O_6$
L-Camphoronic acid
L-Camphoronsaeure
RN: 2385-74-2 **MP** (°C)**:**
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.087E-01	1.110E+02	16	F300	1 0 0 0 2	

1879. $C_9H_{14}O_6$
Triacetin
Propane-1,2,3-triyl triacetate
Enzactin
Vanay
Triacetylglycerol
Glycerol triacetate
RN: 102-76-1 **MP** (°C)**:** –78
MW: 218.21 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.290E-01	7.180E+01	15	F300	1 0 0 0 2	
2.389E-01	5.213E+01	24.50	O005	1 0 2 2 1	
3.118E-02	6.803E+00	ns	F014	0 0 0 0 2	

1880. $C_9H_{15}Br_6O_4P$
Tris-BP
tris(2,3-Dibromopropyl) phosphate
2,3-Dibromo-1-propanol phosphate (3:1)
2,3-Dibromopropyl phosphate
Flamex T 23P
Anfram 3PB
RN: 126-72-7 **MP** (°C)**:** 5.5
MW: 697.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.147E-05	8.000E-03	24	H116	2 1 0 0 2	

1881. $C_9H_{15}Cl_6O_4P$
Fyrol FR-2
tris(1,3-Dichloroisopropyl) phosphate
TCPP
Emulsion 212
TDCPP
PF 38
RN: 13674-87-8 **MP** (°C)**:**
MW: 430.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.624E-05	7.000E-03	24	H116	2 1 0 0 2	

1882. $C_9H_{15}NO_3$
Ecgonine
L-Ekgonin
3-Hydroxy-2-tropane carboxylic acid
RN: 481-37-8 **MP** (°C)**:** 198
MW: 185.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.610E-01	1.780E+02	ns	F300	0 0 0 0 2	

1883. $C_9H_{15}NO_3S$
Captopril
1-((2S)-3-mercapto-2-methylpropionyl)-L-proline
Acenorm
Capoten
Capozide
(*S*)-1-(3-Mercapto-2-methyl-1-oxopropyl)-L-proline
RN: 62571-86-2 **MP** (°C)**:**
MW: 217.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.602E-01	1.000E+02	ns	K444	0 0 0 0 0	
6.348E-01	1.379E+02	ns	S469	0 0 0 0 0	

1884. C_9H_{16}
2,2,5-Trimethyl-3-hexyne
3-Hexyne, 2,2,5-trimethyl-
RN: 17530-23-3 **MP** (°C)**:**
MW: 124.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-04	2.994E-02	25	H039	1 2 2 2 2	

1885. C_9H_{16}
1-Nonyne
n-Heptylacetylene
Heptylacetylene
RN: 3452-09-3 **MP** (°C)**:** –50
MW: 124.23 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.796E-05	7.200E-03	25	M001	2 1 2 2 1	

1886. $C_9H_{16}ClN_4$
G 30451
2-Chloro-4-propylamino-6-isopropylamino-*s*-triazine
RN: 3567-85-9 **MP** (°C)**:**
MW: 215.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.947E-04	4.200E-02	21	B192	0 0 0 0 1	

1887. $C_9H_{16}ClN_5$
Propazine
2-Chloro-4-isopropylamino-6-isopropylamino-*s*-triazine
RN: 139-40-2 **MP** (°C)**:** 213
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.744E-05	8.600E-03	20	B185	0 0 0 0 0	
4.000E-05	9.189E-03	20	B200	1 0 0 0 0	
2.307E-05	5.300E-03	20	C048	2 2 2 2 1	
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.744E-05	8.600E-03	20	M161	1 0 0 0 1	
3.744E-05	8.600E-03	21	B192	0 0 0 0 1	
3.744E-05	8.600E-03	21	G099	2 0 0 1 0	
3.744E-05	8.600E-03	22	M061	1 0 0 0 1	
7.700E-05	1.769E-02	50	G001	1 0 1 1 1	
3.744E-05	8.600E-03	ns	C101	0 0 0 0 1	
4.353E-05	1.000E-02	ns	G041	0 0 0 0 1	
3.744E-05	8.600E-03	ns	J033	0 0 0 0 0	

1888. $C_9H_{16}ClN_5$
Terbuthylazine
Terbutylazine
2-Chloro-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Primatol M
RN: 5915-41-3 **MP** (°C)**:** 178
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.700E-05	8.500E-03	20	M161	1 0 0 0 1	
3.700E-05	8.500E-03	ns	J033	0 0 0 0 0	

1889. $C_9H_{16}ClN_5$
Trietazine
2-Chloro-4-diethylamino-6-ethylamino-*s*-triazine
2-Chloro-4-ethylamino-6-diethylamino-*s*-triazines
RN: 1912-26-1 **MP** (°C)**:** 101
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.706E-05	2.000E-02	20	B185	0 0 0 0 0	
8.706E-05	2.000E-02	21	B192	0 0 0 0 1	
8.706E-05	2.000E-02	21	G099	2 0 0 1 0	
8.706E-05	2.000E-02	25	M161	1 0 0 0 1	
8.706E-05	2.000E-02	ns	J033	0 0 0 0 0	

1890. $C_9H_{16}N_2O_4$
Methyl-2,2-diethylmalonurate
Methyl 2,2-diethylmalonurate
RN: 69577-07-7 **MP** (°C)**:** 112
MW: 216.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	2.379E+00	23	B152	1 2 1 1 1	pH 3.5

1891. $C_9H_{16}N_4OS$
Tebuthiuron
1-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea
Graslan
Spike
Spike 20P
Perflan
RN: 34014-18-1 **MP** (°C)**:** 162.2
MW: 228.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-02	2.300E+00	ns	M161	0 0 0 0 1	

1892. $C_9H_{16}N_8$
2-Azido-4-ethylamino-4-*t*-butylamino-*s*-triazine
WL 9385
RN: 2854-70-8 **MP** (°C)**:** 102.5
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.047E-04	7.200E-02	20	M061	1 0 0 0 1	

1893. $C_9H_{16}O_2$
3-Hydroxy-5-spirocyclohexyltetrahydrofuran
1-Oxaspiro[4.5]decan-3-ol
RN: 29839-61-0 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-01	1.961E+01	rt	B066	0 2 0 0 0	contains impurity

1894. $C_9H_{16}O_2$
g-Nonanolactone
4-Hydroxynonanoic acid lactone
g-*n*-Amylbutyrolactone
g-Pentyl-g-butyrolactone
g-Nonanolide
RN: 104-61-0 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-02	9.217E+00	25	D407	1 0 2 2 2	
5.902E-02	9.221E+00	ns	S460	0 0 0 0 0	

1895. $C_9H_{16}O_2$
3-Hydroxy-2-methyl-5-spirocyclopentyltetrahydrofuran
1-Oxaspiro[4.4]nonan-3-ol, 2-methyl-
RN: 29839-62-1 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E+00	1.667E+02	rt	B066	0 2 0 0 1	

1896. $C_9H_{16}O_4$
Butyl α-acetoxypropionate
Hydracrylic acid, butyl ester, acetate
RN: 5422-69-5 **MP** (°C)**:**
MW: 188.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.200E+00	25	R006	2 2 0 1 1	

1897. $C_9H_{16}O_4$
Azelaic acid
Azelainsaeure
Nonanedioic acid
RN: 123-99-9 **MP** (°C)**:** 106.5
MW: 188.23 **BP** (°C)**:** 287

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.313E-03	1.000E+00	0	L041	1 0 0 1 1	
3.298E-03	6.208E-01	6.99	A340	0 0 0 0 0	
4.513E-03	8.494E-01	12.69	A340	0 0 0 0 0	
7.969E-03	1.500E+00	15	L041	1 0 0 1 1	
6.475E-03	1.219E+00	18.69	A340	0 0 0 0 0	
1.275E-02	2.400E+00	20	F300	1 0 0 0 1	
1.275E-02	2.400E+00	20	L041	1 0 0 1 1	
1.297E-02	2.441E+00	20	M171	1 0 0 0 1	
2.667E-01	5.020E+01	21	B040	1 0 1 1 2	*sic*
9.461E-03	1.781E+00	24.99	A340	0 0 0 0 0	
1.589E-02	2.990E+00	34.69	A340	0 0 0 0 0	
2.391E-02	4.500E+00	35	L041	1 0 0 1 1	
1.858E-02	3.498E+00	42.99	A340	0 0 0 0 0	
4.356E-02	8.200E+00	50	L041	1 0 0 1 1	
2.662E-02	5.010E+00	52.59	A340	0 0 0 0 0	
3.858E-02	7.263E+00	56.99	A340	0 0 0 0 0	
5.124E-02	9.645E+00	61.49	A340	0 0 0 0 0	
7.023E-02	1.322E+01	64.99	A340	0 0 0 0 0	
1.169E-01	2.200E+01	65	F300	1 0 0 0 1	
1.169E-01	2.200E+01	65	L041	1 0 0 1 1	
7.255E-02	1.366E+01	70.99	A340	0 0 0 0 0	
8.355E-02	1.573E+01	74.49	A340	0 0 0 0 0	
1.048E-01	1.972E+01	79.89	A340	0 0 0 0 0	
9.430E-02	1.775E+01	84.49	A340	0 0 0 0 0	
9.440E-03	1.777E+00	rt	H431	0 0 0 0 0	

1898. $C_9H_{16}O_5$
Propanoic acid, 2-[(butoxycarbonyl)oxy]-, methyl ester
Propanoic acid, 2-[(methoxycarbonyl)oxy]-, butyl ester
RN: **MP** (°C)**:**
MW: 204.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.798E-03	1.797E+00	25	R007	0 0 0 0 0	

1899. $C_9H_{17}ClN_3O_3PS$
Isazophos
Diethyl *O*-(5-chloro-1-(1-methylethyl)-1H-1,2,4-triazol-3-yl) phosphorothioate
Miral
Triumph
CGA-12223
RN: 42509-80-8 **MP** (°C)**:**
MW: 313.74 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.500E-01	20	E048	1 2 1 1 2	
4.781E-04	1.500E-01	20	M161	1 0 0 0 1	

1900. $C_9H_{17}NOS$
Molinate
S-Ethyl hexahydro-1H-azepine-1-carbothioate
Hydram
Carbothialate, ethyl-1-hexa-methylene imine-
Poperidinecarbothioic acid, *S*-ethyl ester
RN: 2212-67-1 **MP** (°C)**:**
MW: 187.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.271E-03	8.000E-01	20	B200	1 0 0 0 2	
4.271E-03	8.000E-01	21	M161	1 0 0 0 2	
4.698E-03	8.800E-01	22	K137	1 1 2 1 0	
4.698E-03	8.800E-01	25	P434	0 0 0 0 0	
<5.33E-03	<9.99E-01	ns	B185	0 0 0 0 0	
4.869E-03	9.120E-01	ns	F019	0 0 0 0 2	
5.334E-03	9.990E-01	ns	M061	0 0 0 0 0	

1901. $C_9H_{17}NO_3$
Diethylaceturethane
Detonal
RN: **MP** (°C)**:**
MW: 187.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.796E-02	5.236E+00	ns	O021	0 2 0 0 0	

1902. $C_9H_{17}NO_4$
3,3-Dihydroxy-2,2,5,5-tetramethyl-4-carbamyltetrahydrofuran
3-Furamide, tetrahydro-4,4-dihydroxy-2,2,5,5-tetramethyl-
RN: 29839-68-7 **MP** (°C)**:**
MW: 203.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.473E-01	9.091E+01	rt	B066	0 2 0 0 1	

1903. $C_9H_{17}N_5O$
Atratone
2-Methoxy-4-ethylamino-6-isopropylamino-*s*-triazine
2-Methoxy-4-ethylamino-6-isopropylamino-*s*-triazines
RN: 1610-17-9 **MP** (°C)**:**
MW: 211.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.520E-03	1.800E+00	20	B185	0 0 0 0 0	
8.520E-03	1.800E+00	20	M061	1 0 0 0 2	
8.520E-03	1.800E+00	21	B192	0 0 0 0 2	
8.520E-03	1.800E+00	21	G099	2 0 0 1 0	
7.905E-03	1.670E+00	25	H073	2 1 1 2 2	
1.240E-02	2.620E+00	50	G001	1 0 1 1 2	
9.448E-03	1.996E+00	ns	B100	0 0 0 0 0	
8.520E-03	1.800E+00	ns	C101	0 0 0 0 1	
7.829E-03	1.654E+00	ns	J033	0 0 0 0 0	

1904. $C_9H_{17}N_5S$

Ametryn
(2-Methylthio-4-ethylamino-6-isopropylamino-*s*-triazine
Ametryne
N-Ethyl-*N′*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
Ametrex

RN: 834-12-8 **MP** (°C)**:** 84
MW: 227.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-04	1.841E-01	20	B200	1 0 0 0 1	
8.358E-04	1.900E-01	20	F311	1 2 2 2 1	
8.138E-04	1.850E-01	20	M161	1 0 0 0 2	
9.194E-04	2.090E-01	25	H073	2 1 1 2 2	
1.660E-03	3.774E-01	50	G001	1 0 1 1 2	
8.138E-04	1.850E-01	ns	C101	0 0 0 0 1	
8.490E-04	1.930E-01	ns	J033	0 0 0 0 0	

1905. C_9H_{18}

1-Nonene
α-Nonene
1-*n*-Nonene
n-Non-1-ene

RN: 124-11-8 **MP** (°C)**:** –81
MW: 126.24 **BP** (°C)**:** 146.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.850E-06	1.117E-03	25	M342	1 0 1 1 2	

1906. C_9H_{18}

1,1,3-Trimethylcyclohexane
Cyclogeraniolane

RN: 3073-66-3 **MP** (°C)**:** –65.7
MW: 126.24 **BP** (°C)**:** 136.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-05	1.770E-03	25	K119	1 0 0 0 2	
1.402E-05	1.770E-03	25	P051	2 1 1 2 2	
1.402E-05	1.770E-03	25.00	P007	2 1 2 2 2	

1907. $C_9H_{18}N_2O_2S$
Thiofanox
3,3-Dimethyl-1-(methylthio)-2-butanone *O*-((methylamino)carbonyl)oxime
Thiophanox
DS-15647
Dacamox
RN: 39196-18-4 **MP** (°C)**:** 57
MW: 218.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	5.200E+00	22	M161	1 0 0 0 1	

1908. $C_9H_{18}N_2O_4$
Meprobamate
2-Methyl-2-propyl-1,3-propanediol dicarbamate
Deprol
Meprospan
Miltown
Pathibamate
RN: 57-53-4 **MP** (°C)**:** 104
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.841E-02	6.200E+00	25	C039	1 2 2 1 1	form II
1.512E-02	3.300E+00	25	C039	1 2 2 1 1	form I
1.512E-02	3.300E+00	25	D082	1 0 1 0 1	
3.757E-02	8.200E+00	30	C039	1 2 2 1 1	form II
1.970E-02	4.300E+00	30	C039	1 2 2 1 1	form I
2.612E-02	5.700E+00	35	C039	1 2 2 1 1	form I
4.857E-02	1.060E+01	35	C039	1 2 2 1 2	form II
3.391E-02	7.400E+00	40	C039	1 2 2 1 1	form I
5.865E-02	1.280E+01	40	C039	1 2 2 1 2	form II

1909. $C_9H_{18}N_3S_6Fe$
Ferbam
tris(Dimethyldithiocarbamate)iron
Knockmate
Ferbeck
Hexaferb
Trifungol
RN: 14484-64-1 **MP** (°C)**:**
MW: 416.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.881E-04	1.200E-01	rt	I314	0 0 0 0 0	
3.121E-04	1.300E-01	rt	M161	0 0 0 0 2	

1910. $C_9H_{18}N_6$
Altretamine
Hexamethylmelamine
2,4,6-tris(Dimethylamino)-1,3,5-triazine
HMM
Hexastat
Hemel
RN: 645-05-6 **MP** (°C)**:** 172.0
MW: 210.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.846E-04	8.088E-02	25	B386	0 0 0 0 0	
4.327E-04	9.100E-02	25	C051	1 2 1 1 1	pH 7
4.150E-04	8.727E-02	25	K043	2 0 0 0 0	extrapolated

1911. $C_9H_{18}N_6$
1,3,5-Triazine-2,4,6-triamine, *N,N′,N″*-Triethyl-
*N*2,*N*4,*N*6-Triethylmelamine
tris(Ethylamino)-1,3,5-triazine
2,4,6-tris(Ethylamino)-1,3,5-triazine
2,4,6-tris(Ethylamino)-*s*-triazine
N,N′,N″-Triethyl-1,3,5-triazine-2,4,6-triamine
RN: 16268-92-1 **MP** (°C)**:**
MW: 210.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.318E-03	1.539E+00	25	B386	0 0 0 0 0	

1912. $C_9H_{18}N_6O$
N-Methylolpentamethylmelamine
N-(Hydroxymethyl)pentamethylmelamine
(Hydroxymethyl)pentamethylmelamine
RN: 16269-01-5 **MP** (°C)**:** 121.0
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.977E-03	9.000E-01	25	C051	1 2 1 1 0	pH 7, unstable in water

1913. $C_9H_{18}N_6O$
Ethanol, 2-[[4,6-bis(dimethylamino)-*s*-triazin-2-yl]amino]-
Ethanol, 2-[[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]amino]-
RN: 31482-09-4 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-02	2.562E+00	25	B386	0 0 0 0 0	

1914. $C_9H_{18}N_6O_3$
*N*2,*N*4,*N*6-Trimethyl-*N*2,*N*4,*N*6-trimethylolmelamine
N,N′,N″-Trimethyl-*N,N′,N″*-trimethylolmelamine
Trimelamol
CB 10-375
RN: 64124-21-6 **MP** (°C)**:** 129
MW: 258.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	9.040E+00	25	C051	1 2 1 1 2	pH 7

1915. $C_9H_{18}O$
Nonyl aldehyde
n-Nonanal
RN: 124-19-6 **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:** 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.749E-04	9.600E-02	25	A049	1 0 0 0 1	

1916. $C_9H_{18}O$
5-Nonanone
Dibutyl ketone
RN: 502-56-7 **MP** (°C)**:** –50
MW: 142.24 **BP** (°C)**:** 186.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.078E-01	10	G032	1 2 1 1 2	
1.800E-03	2.560E-01	25	K012	1 0 0 0 1	
2.550E-03	3.627E-01	30	G032	1 2 1 1 2	
2.430E-03	3.457E-01	50	G032	1 2 1 1 2	

1917. $C_9H_{18}O$
3-Hydroxy-2,3,4,5,5-pentamethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-01	9.091E+01	rt	B066	0 2 0 0 1	

1918. $C_9H_{18}O$

2,6-Dimethyl-4-heptanone
Diisobutyl ketone
RN: 108-83-8 **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	2.633E+00	23.50	O005	2 0 2 2 2	

1919. $C_9H_{18}O$

2-Nonanone
Nonan-2-one
RN: 821-55-6 **MP** (°C)**:** –21
MW: 142.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-03	1.900E-01	25	L450	0 0 0 0 0	

1920. $C_9H_{18}O_2$

3-Hydroxy-2-isopropyl-5,5-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2-isopropyl-5,5-dimethyl-
RN: 29839-66-5 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.009E-01	4.762E+01	rt	B066	0 2 0 0 0	

1921. $C_9H_{18}O_2$

Pelargonic acid
1-Octanecarboxylic acid
Nonylic acid
n-Nonanoic acid
RN: 112-05-0 **MP** (°C)**:** 12
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.847E-04	1.400E-01	0	B136	1 0 2 1 1	
1.795E-03	2.840E-01	20	B136	1 0 2 1 2	
1.643E-03	2.599E-01	20.0	R001	1 1 1 1 1	
2.003E-03	3.170E-01	30	B136	1 0 2 1 2	
1.340E-03	2.120E-01	30	E005	2 1 1 2 2	
2.022E-03	3.199E-01	30.0	R001	1 1 1 1 1	
2.496E-03	3.950E-01	40	B136	1 0 2 1 2	
1.403E-03	2.220E-01	40	E005	2 1 1 2 2	
2.591E-03	4.100E-01	45	B136	1 0 2 1 1	
2.590E-03	4.098E-01	45.0	R001	1 1 1 1 1	

(*continued*)

1921. $C_9H_{18}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-03	2.640E-01	50	E005	2 1 1 2 2	
3.223E-03	5.100E-01	60	B136	1 0 2 1 1	
1.890E-03	2.990E-01	60	E005	2 1 1 2 2	
3.221E-03	5.097E-01	60.0	R001	1 1 1 1 1	
8.846E-04	1.400E-01	.0	R001	1 1 1 1 1	

1922. $C_9H_{18}O_2$
Methyl octanoate
Methyl caprylate
Methyl octylate
RN: 111-11-5 **MP** (°C)**:** –37
MW: 158.24 **BP** (°C)**:** 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.069E-04	6.440E-02	20	M337	2 1 2 2 2	

1923. $C_9H_{18}O_2$
3-Hydroxy-5-propyl-2,5-dimethyltetrahydrofuran
3-Furanol, 2,5-dimethyltetrahydro-5-propyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-01	2.913E+01	rt	B066	0 2 0 0 0	

1924. $C_9H_{18}O_2$
3-Hydroxy-5-methyl-5-isobutyltetrahydrofuran
3-Furanol, 5-isobutyltetrahydro-5-methyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1925. $C_9H_{18}O_2$
3-Hydroxy-5-methyl-5-butyltetrahydrofuran
3-Furanol, 5-butyltetrahydro-5-methyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.518E-02	3.984E+00	rt	B066	0 2 0 0 0	

1926. $C_9H_{18}O_2$
3-Hydroxy-3-ethyl-2,2,5-trimethyltetrahydrofuranol
3-Furanol, 3-ethyltetrahydro-2,2,5-trimethyl-
RN: 29839-58-5 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.134E-01	6.542E+01	rt	B066	0 2 0 0 0	

1927. $C_9H_{18}O_2$
3-Hydroxy-2-methyl-2,5-diethyltetrahydrofuran
3-Furanol, 2,5-diethyltetrahydro-2-methyl-
RN: 29839-64-3 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	1.961E+01	rt	B066	0 2 0 0 0	

1928. $C_9H_{18}O_2$
3-Hydroxy-2,2,4,5,5-pentamethyltetrahydrofuran
3-Furanol, tetrahydro-2,2,4,5,5-pentamethyl-
RN: 29839-76-7 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1929. $C_9H_{18}O_2$
Butyl valerate
n-Butyl pentanoate
Butyl valerianate
RN: 591-68-4 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:** 186–187

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	8.387E-02	25	K012	1 0 0 0 1	

1930. $C_9H_{18}O_2$
Pentyl butyrate
n-Amyl *n*-butyrate
Pentyl *n*-butanoate
RN: 540-18-1 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	1.741E-01	20	S006	1 0 0 0 1	

1931. $C_9H_{18}O_2$
3-Hydroxy-2-methyl-5,5-diethyltetrahydrofuran
3-Furanol, 5,5-diethyltetrahydro-2-methyl-
RN: 6744-54-3 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.144E-02	4.975E+00	rt	B066	0 2 0 0 0	

1932. $C_9H_{18}O_3$
2,2-Diethyl-5-methyl-tetrahydrofuran-3,4-diol
3,4-Furandiol, 2,2-diethyltetrahydro-5-methyl-
RN: 31889-35-7 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.565E-01	1.667E+02	rt	B066	0 2 0 0 1	

1933. $C_9H_{18}O_3$
n-Propyl β-*n*-propoxypropionate
Propanoic acid, 3-propoxy-, propyl ester
RN: 14144-41-3 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-02	3.587E+00	25	R034	0 0 0 0 1	

1934. $C_9H_{18}O_3$
n-Amyl β-methoxypropionate
Pentyl 3-methoxypropionate
RN: 10500-16-0 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-02	2.892E+00	25	R034	0 0 0 0 1	

1935. $C_9H_{18}O_3$
1,3-Dioxolane-4-methanol, 2-butyl-2-methyl
RN: 5694-76-8 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.380E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

1936. $C_9H_{18}O_3$
n-Butyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, butyl ester
RN: 14144-35-5 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.287E-02	3.984E+00	25	D002	1 2 1 1 1	

1937. $C_9H_{18}O_3$
Hexyl lactate
Propanoic acid, 2-hydroxy-, hexyl ester
RN: 20279-51-0 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.700E+00	25	R006	2 2 0 1 1	

1938. $C_9H_{19}NOS$
Eptam
EPTC
Ethyl *N,N′*-di-*n*-propylthiolcarbamate
S-Ethyl dipropylthiocarbamate
S-Ethyl *N,N*-di-*n*-propylthiocarbamate
RN: 759-94-4 **MP** (°C)**:** <25
MW: 189.32 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-03	6.360E-01	3	G319	0 0 0 0 0	
1.954E-03	3.700E-01	20	B200	1 0 0 0 2	
1.981E+01	3.750E+03	20	F019	1 0 0 0 2	*sic*
1.981E-03	3.750E-01	20	M061	1 0 0 0 2	
1.928E-03	3.650E-01	20	M161	1 0 0 0 2	
4.170E+00	7.895E+02	25	B185	0 0 0 0 0	*sic*
1.981E-03	3.750E-01	25	G319	0 0 0 0 0	
1.981E-03	3.750E-01	25	M131	0 0 0 0 2	
2.123E-03	4.020E-01	28	H109	1 0 0 0 2	
1.981E-03	3.750E-01	ns	V414	0 0 0 0 0	

1939. $C_9H_{19}NO_2$
n-Octyl carbamate
Carbamic acid, octyl ester
RN: 2029-64-3 **MP** (°C)**:** 67
MW: 173.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	8.663E-02	37	H006	1 2 2 1 0	

1940. $C_9H_{19}O_3$
3-Hydroxy-4-methylol-2,2,5,5-tetramethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 175.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.119E-01	1.961E+01	rt	B066	0 2 0 0 0	

1941. C_9H_{20}
3,3-Diethylpentane
Tetraethylmethane
RN: 1067-20-5 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-06	1.212E-03	25	D346	0 0 0 0 0	

1942. C_9H_{20}
2,5-Dimethylheptane
RN: 2216-30-0 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1943. C_9H_{20}
3-Methyloctane
Octane, 3-methyl-
RN: 2216-33-3 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.237E-06	8.000E-04	23	C332	0 0 0 0 0	

1944. C_9H_{20}
2-Methyl-4-ethylhexane
RN: 3074-75-7 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E-06	3.590E-04	ns	S460	0 0 0 0 0	

1945. C_9H_{20}
2,2,3-Trimethylhexane
RN: 16747-25-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-06	3.623E-04	ns	S460	0 0 0 0 0	

1946. C_9H_{20}
2,4-Dimethylheptane
RN: 2213-23-2 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 133

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.938E-06	3.768E-04	ns	S460	0 0 0 0 0	

1947. C_9H_{20}
2,2,5-Trimethylhexane
Hexane, 2,2,5-trimethyl-
RN: 3522-94-9 **MP** (°C)**:** –120
MW: 128.26 **BP** (°C)**:** 124.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.159E-06	7.900E-04	0	P003	2 2 2 2 1	
8.966E-06	1.150E-03	25	M001	2 1 2 2 2	
4.210E-06	5.400E-04	25	P003	2 2 2 2 1	

1948. C_9H_{20}
2,2-Dimethylheptane
RN: 1071-26-7 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	3.592E-04	ns	S460	0 0 0 0 0	

1949. C_9H_{20}
Nonane
n-Nonan
RN: 111-84-2 **MP** (°C)**:** –53
MW: 128.26 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.72E-05	<2.20E-03	20	M337	2 1 2 2 1	
9.512E-07	1.220E-04	25	K119	1 0 0 0 2	
1.715E-06	2.200E-04	25	M003	1 0 2 2 2	
1.333E-06	1.710E-04	25	T423	0 0 0 0 0	
9.512E-07	1.220E-04	25.0	P051	2 1 1 2 2	
9.512E-07	1.220E-04	25.00	P007	2 1 2 2 2	
2.409E-06	3.090E-04	69.7	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.1	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.10	P007	2 1 2 2 2	
1.325E-05	1.700E-03	121.3	P051	2 1 1 2 2	
1.325E-05	1.700E-03	121.30	P007	2 1 2 2 2	
3.953E-05	5.070E-03	136.6	P051	2 1 1 2 2	
3.953E-05	5.070E-03	136.60	P007	2 1 2 2 2	

1950. C_9H_{20}
4,4-Dimethylheptane
RN: 1068-19-5 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-06	3.335E-04	ns	S460	0 0 0 0 0	

1951. C_9H_{20}
2,6-Dimethylheptane
RN: 1072-05-5 **MP** (°C)**:** –103
MW: 128.26 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.594E-06	3.327E-04	ns	S460	0 0 0 0 0	

1952. C_9H_{20}
3,5-Dimethylheptane
RN: 926-82-9 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1953. C_9H_{20}
3-Ethylheptane
RN: 15869-80-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.714E-06	2.198E-04	ns	S460	0 0 0 0 0	

1954. C_9H_{20}
4-Ethylheptane
RN: 2216-32-2 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-06	2.422E-04	ns	S460	0 0 0 0 0	

1955. C_9H_{20}
2,3-Dimethylheptane
RN: 3074-71-3 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.959E-06	2.512E-04	ns	S420	0 0 0 0 0	

1956. C_9H_{20}
2,3,4-Trimethylhexane
RN: 921-47-1 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.113E-06	2.711E-04	ns	S460	0 0 0 0 0	

1957. C_9H_{20}
3-Ethyl-2-methylhexane
2-Methyl-3-ethylhexane
RN: 16789-46-1 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E-06	2.871E-04	ns	S460	0 0 0 0 0	

1958. C_9H_{20}
3,3-Dimethylheptane
RN: 4032-86-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-06	3.028E-04	ns	S460	0 0 0 0 0	

1959. C_9H_{20}
4-Methyloctane
4-Metylooktan
RN: 2216-34-4 **MP** (°C)**:** –113
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.966E-07	1.150E-04	25	K119	1 0 0 0 2	
8.966E-07	1.150E-04	25	P051	2 1 1 2 2	
8.966E-07	1.150E-04	25.00	P007	2 1 2 2 2	

1960. $C_9H_{20}NO_3PS_2$
Fostion
FAC 20
O,O-Diethyl *S*-(*N*-isopropylcarbamylmethyl) dithiophosphate
Prothoate
RN: 2275-18-5 **MP** (°C)**:** 24.5
MW: 285.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.761E-03	2.500E+00	20	M161	1 0 0 0 1	

1961. $C_9H_{20}O$
2,6-Dimethyl-4-heptanol
Diisobutylcarbinol
RN: 108-82-7 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.925E-03	9.990E-01	25	C093	2 1 1 1 1	

1962. $C_9H_{20}O$
n-Nonyl alcohol
Nonanol
RN: 143-08-8 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.340E-04	1.347E-01	20	H330	0 0 0 0 0	
9.700E-04	1.399E-01	25	K025	2 2 1 1 2	

1963. $C_9H_{20}O$
3-Ethyl-3-heptanol
RN: 19780-41-7 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	5.485E-01	ns	S460	0 0 0 0 0	

1964. $C_9H_{20}O$
2,6-Dimethyl-3-heptanol
RN: 19549-73-6 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.097E-03	4.468E-01	ns	S460	0 0 0 0 0	

1965. $C_9H_{20}O$
3-Nonanol
Hexyl ethyl carbinol
Ethyl *n*-hexyl carbinol
RN: 624-51-1 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.999E-03	2.884E-01	ns	J300	0 0 0 0 0	

1966. $C_9H_{20}O$

3,5,5-Trimethylhexanol
3.,5,5-Trimethyl hexanol
Nonylol
3,5,5-Trimethyl-1-hexanol
RN: 3452-97-9 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.501E-01	20	H330	0 0 0 0 0	
3.099E-03	4.470E-01	ns	J300	0 0 0 0 0	

1967. $C_9H_{20}O$

Methyl-octyl-alcohol
2-Nonanol
Heptylmethylcarbinol
Methyl *n*-heptyl carbinol
RN: 628-99-9 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.00E-03	<5.77E-01	25	F044	1 0 0 0 0	

1968. $C_9H_{21}N$

Tripropylamine
Tri-*n*-propylamine
N,N-Dipropylpropanamine
N,N-Dipropyl-1-propanamine
RN: 102-69-2 **MP** (°C)**:** –93.5
MW: 143.27 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E-03	7.473E-01	25.04	V013	2 2 2 2 2	

1969. $C_9H_{21}O_2PS_3$

Terbufos
O,O-Diethyl *S*-(((1,1-dimethylethyl)thio)methyl) phosphorodithoic acid
Counter 15G
Contraven
ST 100
RN: 13071-79-9 **MP** (°C)**:**
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-05	5.500E-03	19	B169	2 1 1 1 1	
1.758E-05	5.070E-03	24	F179	2 2 2 2 2	
1.907E-05	5.500E-03	ns	B325	0 1 0 0 1	

(*continued*)

1969. $C_9H_{21}O_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	1.000E-02	ns	M110	0 0 0 0 0	EFG
4.334E-05	1.250E-02	ns	M161	0 0 0 0 0	

1970. $C_9H_{21}O_3P$
Dibutyl methyl phosphonate
Di-*n*-butyl methanephosphonate
RN: 2404-73-1 **MP** (°C)**:**
MW: 208.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.842E-02	8.000E+00	25	B070	1 2 0 1 0	

1971. $C_9H_{21}O_3PS_3$
S-Ethylsulphinylmethyl *O,O*-di-isopropyl phosphorodithioate
O,O-Diisopropyl *S*-[(ethylsulfinyl)methyl] dithiophosphate
Aphidan
PSP 204
IPSP
RN: 5827-05-4 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E-03	1.500E+00	15	M161	1 0 0 0 1	

1972. $C_9H_{21}O_3PS_3$
Terbufos sulfoxide
Phosphorodithioic acid, *S*-[[(1,1-dimethylethyl)sulfinyl]methyl] *O,O*-diethyl ester
RN: 10548-10-4 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.61E-03	>1.10E+00	ns	B325	0 1 0 0 1	

1973. $C_9H_{21}O_4P$
Tripropyl phosphate
Tri-*n*-propyl phosphate
RN: 513-08-6 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	6.951E+00	30	V300	2 2 0 1 0	

1974. $C_9H_{21}O_4P$
Dibutyl methyl phosphate
Methyl dibutyl phosphate
RN: 7242-59-3 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.166E-02	7.100E+00	25	B070	1 2 2 1 1	

1975. $C_9H_{21}O_4P$
Diethyl amyl phosphate
O,O-Diethyl *O*-pentyl phosphate
Diethyl pentyl phosphate
RN: 20195-08-8 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.345E-02	7.500E+00	25	B070	1 2 0 1 1	

1976. $C_9H_{21}O_4PS_3$
Terbufos sulfone
Phosphorodithioic acid, *S*-[[(1,1-dimethylethyl)sulfonyl]methyl] *O,O*-diethyl ester
Counter sulfone
AC 94320
RN: 56070-16-7 **MP** (°C)**:**
MW: 320.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-03	4.078E-01	18.50	B169	2 0 1 1 2	
1.273E-03	4.078E-01	ns	B325	0 1 0 0 1	

1977. $C_9H_{22}O_4P_2S_4$
Ethion
O,O,O,O-Tetraethyl *S,S*-methylene bisphosphorodithioate
Nialate
Ethanox
Diethion
Hylemox
RN: 563-12-2 **MP** (°C)**:** –25
MW: 384.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-06	5.700E-04	10	B324	0 0 0 0 0	
1.483E-06	5.702E-04	10	B324	0 0 0 0 0	
2.861E-06	1.100E-03	19.50	B169	2 2 1 1 1	
1.769E-06	6.801E-04	20	B324	0 0 0 0 0	
1.769E-06	6.800E-04	20	B324	0 0 0 0 0	

(*continued*)

1977. $C_9H_{22}O_4P_2S_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-06	7.601E-04	30	B324	0 0 0 0 0	
1.977E-06	7.600E-04	30	B324	0 0 0 0 0	

1978. $C_{10}H_4Cl_2O_2$

Dichlone
2,3-Dichloro-1,4-naphthalenedione
Phygon XL
Phygon
Phygon paste
USR 604

RN: 117-80-6 **MP** (°C)**:**
MW: 227.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.404E-07	1.000E-04	25	M161	1 0 0 0 0	
3.083E-05	7.000E-03	ns	B160	0 0 0 0 0	
4.404E-06	1.000E-03	ns	B185	0 0 0 0 0	

1979. $C_{10}H_5ClN_2O_4$

1-Chloro-2,4-dinitronaphthalene
2,4-Dinitro-1-naphthyl chloride
2,4-Dinitrochloronaphthalene
2,4-Dinitro-1-chloronaphthalene

RN: 2401-85-6 **MP** (°C)**:** 148
MW: 252.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-06	1.000E-03	25	M061	1 0 0 0 0	

1980. $C_{10}H_5Cl_7$

Heptachlor
1,4,5,6,7,8,8-Heptachloro-3α,4,7,7α-tetrahydro-4,7-methano-1H-indene
3-Chlorochlordene
Tetrahydro
Rhodiachlor
3,4,5,6,7,8,8α-Heptachlorodicyclopentadiene

RN: 76-44-8 **MP** (°C)**:** 95.5
MW: 373.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-07	1.000E-04	15	B083	2 2 1 2 2	particle size 5 µm
4.786E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.822E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 µm

(*continued*)

1980. $C_{10}H_5Cl_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-07	5.600E-05	25	I308	0 0 0 0 0	
1.500E-07	5.600E-05	26.5	P027	1 1 2 2 1	
1.500E-07	5.600E-05	27	M161	0 0 0 0 1	
8.438E-07	3.150E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.313E-06	4.900E-04	45	B083	2 2 1 2 2	particle size 5 µm
8.036E-08	3.000E-05	ns	K138	0 0 0 0 2	
1.875E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
4.822E-07	1.800E-04	ns	V414	0 0 0 0 0	

1981. $C_{10}H_5Cl_7O$

Heptachlor epoxide
1,4,5,6,7,8,8-Heptachloro-2,3-epoxy-3α,4,7,7α-tetrahydro-4,7-methanoindan
Hepachlor epoxide

RN: 1024-57-3 **MP** (°C)**:** 160
MW: 389.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-07	1.100E-04	15	B083	2 2 1 2 2	particle size 5 µm
5.137E-07	2.000E-04	25	B083	2 2 1 2 2	particle size 5 µm
5.137E-07	2.000E-04	25	I308	0 0 0 0 0	
8.990E-07	3.500E-04	25	W025	1 0 2 2 2	
8.990E-07	3.500E-04	26.5	P027	1 1 2 2 1	
8.990E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.541E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.798E-06	7.000E-04	ns	M110	0 0 0 0 0	EFG
5.137E-07	2.000E-04	ns	V414	0 0 0 0 0	

1982. $C_{10}H_5N_3O_6$

1,3,8-Trinitronaphthalene
1,3,8-Trinitronaphthalin

RN: 2364-46-7 **MP** (°C)**:**
MW: 263.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-05	1.800E-02	15	F300	1 0 0 0 1	

1983. $C_{10}H_5N_3O_6$

1,4,5-Trinitronaphthalene
1,4,5-Trinitronaphthalin

RN: 2243-95-0 **MP** (°C)**:**
MW: 263.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.520E-04	4.000E-02	15	F300	1 0 0 0 1	

1984. $C_{10}H_6Br_2$
2,3-Dibromonaphthalene
Naphthalene, 2,3-dibromo-
RN: 13214-70-5 **MP** (°C)**:**
MW: 285.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-07	5.497E-05	4	D351	1 2 1 1 2	
4.778E-07	1.366E-04	25	D351	1 2 1 1 2	
1.222E-06	3.495E-04	40	D351	1 2 1 1 2	

1985. $C_{10}H_6Br_2$
1,4-Dibromonaphthalene
Naphthalene, 1,4-dibromo-
RN: 83-53-4 **MP** (°C)**:** 80–82
MW: 285.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.333E-07	1.239E-04	4	D351	1 2 1 1 2	
1.217E-06	3.479E-04	25	D351	1 2 1 1 2	
3.006E-06	8.595E-04	40	D351	1 2 1 1 2	

1986. $C_{10}H_6Cl_2$
1,4-Dichloronaphthalene
Naphthalene, 1,4-dichloro-
RN: 1825-31-6 **MP** (°C)**:**
MW: 197.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-06	2.628E-04	4	D351	1 2 1 1 2	
4.389E-06	8.649E-04	25	D351	1 2 1 1 2	
1.122E-05	2.212E-03	40	D351	1 2 1 1 2	

1987. $C_{10}H_6Cl_4O_3S$
Glenbar
O,S-Dimethyl tetrachlorothioterephthalate
RN: 3765-57-9 **MP** (°C)**:** 161
MW: 348.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.437E-06	5.000E-04	22	B200	1 0 0 0 0	
1.034E-06	3.600E-04	ns	M061	0 0 0 0 1	

1988. $C_{10}H_6Cl_4O_4$
Dimethyl tetrachloroterephthalate
DCPA
RN: 1861-32-1 **MP** (°C)**:** 156
MW: 331.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-06	5.000E-04	25	B200	1 0 0 0 0	
<1.51E-06	<5.00E-04	25	M161	1 0 0 0 0	
<1.51E-06	<5.00E-04	ns	B185	0 0 0 0 0	
1.506E-06	5.000E-04	ns	V414	0 0 0 0 0	

1989. $C_{10}H_6Cl_6$
Chlordene
4,5,6,7,8,8-Hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
RN: 3734-48-3 **MP** (°C)**:** –62
MW: 338.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.281E-06	7.730E-04	26.70	L071	1 2 0 1 2	

1990. $C_{10}H_6Cl_6O$
1-Hydroxychlordene
1-Hydroxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetra-hydro-4,7-methanoindene
RN: 2597-11-7 **MP** (°C)**:** 194
MW: 354.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.469E-06	1.231E-03	26.70	L071	1 2 0 1 2	

1991. $C_{10}H_6Cl_6O$
Chlordene epoxide
2,3-Epoxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
Chlordene hydroxide
4,7-Methano-1H-inden-1-ol, 4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-
RN: 6058-23-7 **MP** (°C)**:** 215
MW: 354.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.829E-06	1.359E-03	26.70	L071	1 2 0 1 2	

1992. $C_{10}H_6Cl_6O_2$
1-Hydroxychlordene epoxide
1-Hydroxy-2,3-epoxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
RN: 24009-06-1 **MP** (°C)**:**
MW: 370.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.391E-06	2.741E-03	26.70	L071	1 1 1 1 2	

1993. $C_{10}H_6Cl_8$
cis-Chlordane
(1α,2α,3aα,4β,7β,7aα)-1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1α,2α,3aα,4β,7β,7aα)
α-Chlordane
RN: 5103-71-9 **MP** (°C)**:**
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1994. $C_{10}H_6Cl_8$
trans-Chlordane
(1α,2β,3aα,4β,7β,7aα)-1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1α,2β,3aα,4β,7β,7aα)-
β-Chlordane
RN: 5103-74-2 **MP** (°C)**:**
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1995. $C_{10}H_6Cl_8$
Chlordane
1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3α,4,7,7α-tetrahydroindane
Octachlor
Velsicol 1068
Toxichlor
Ortho-Klor
RN: 57-74-9 **MP** (°C)**:** 105
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-07	5.657E-05	24.99	K436	0 0 0 0 0	
4.515E-06	1.850E-03	25	W025	1 0 2 2 2	
1.367E-07	5.600E-05	ns	K138	0 0 0 0 2	

(*continued*)

1995. $C_{10}H_6Cl_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
1.367E-07	5.600E-05	ns	S187	0 2 2 1 1	
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1996. $C_{10}H_6FN_3O_3$
3-Nicotinoyl-5-fluorouracil
RN: **MP** (°C)**:**
MW: 235.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E-02	2.700E+00	22	B332	1 1 0 0 1	pH 4.0

1997. $C_{10}H_6N_2O_4$
1,8-Dinitronaphthalene
1,8-Dinitronaphthalin
RN: 602-38-0 **MP** (°C)**:** 107
MW: 218.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-04	3.400E-02	15	F300	1 0 0 0 1	

1998. $C_{10}H_6N_2O_4$
1,5-Dinitronaphthalene
1,5-Dinitronaphthalin
RN: 605-71-0 **MP** (°C)**:** 216.5
MW: 218.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.658E-04	5.800E-02	12	F300	1 0 0 0 1	

1999. $C_{10}H_6O_8$
Pyromellitic acid
1,2,4,5-Benzenetetracarboxylic acid
Benzol-tetracarbonsaeure-(1,2,4,5)
RN: 89-05-4 **MP** (°C)**:**
MW: 254.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-02	1.400E+01	16	F300	1 0 0 0 2	

2000. $C_{10}H_7Br$
1-Bromonaphthalene
Naphthalene, 1-bromo-
RN: 90-11-9 **MP** (°C)**:** 6.2
MW: 207.08 **BP** (°C)**:** 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.383E-05	9.077E-03	4	D351	1 2 1 1 2	
4.733E-05	9.802E-03	10	D351	1 2 1 1 2	
4.500E-05	9.318E-03	21	A057	2 1 2 2 1	
6.444E-05	1.334E-02	25	D351	1 2 1 1 2	
9.166E-05	1.898E-02	40	D351	1 2 1 1 2	
6.000E-05	1.242E-02	ns	L060	0 0 0 0 0	
9.120E-05	1.889E-02	ns	S460	0 0 0 0 0	

2001. $C_{10}H_7Br$
2-Bromonaphthalene
Naphthalene, 2-bromo-
RN: 580-13-2 **MP** (°C)**:** 53.5
MW: 207.08 **BP** (°C)**:** 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.831E-03	4	D351	1 2 1 1 2	
3.883E-05	8.041E-03	25	D351	1 2 1 1 2	
7.611E-05	1.576E-02	40	D351	1 2 1 1 2	
4.000E-05	8.283E-03	ns	L060	0 0 0 0 0	

2002. $C_{10}H_7Cl$
β-Chloronaphthalene
2-Chloronaphthalene
RN: 91-58-7 **MP** (°C)**:** 59.5
MW: 162.62 **BP** (°C)**:** 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-06	<1.00E-03	30	M311	1 1 2 2 0	
8.000E-05	1.301E-02	ns	L060	0 0 0 0 0	

2003. $C_{10}H_7Cl$
1-Chloronaphthalene
α-Chloronaphthalene
1-Naphthyl chloride
RN: 90-13-1 **MP** (°C)**:** –20
MW: 162.62 **BP** (°C)**:** 259.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.23E-04	<2.00E-02	ns	L060	0 0 0 0 2	
1.164E-04	1.893E-02	ns	S460	0 0 0 0 0	

2004. $C_{10}H_7I$
α-Iodonaphthalene
1-Iodonaphthalene
RN: 90-14-2 **MP** (°C)**:**
MW: 254.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.114E-03	ns	L060	0 0 0 0 1	average
2.818E-05	7.161E-03	ns	S460	0 0 0 0 0	

2005. $C_{10}H_7NO_2$
1-Nitronaphthalene
1-Nitro-naphthalin
RN: 86-57-7 **MP** (°C)**:** 59.5
MW: 173.17 **BP** (°C)**:** 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-04	5.000E-02	18	F300	1 0 0 0 1	

2006. $C_{10}H_7NO_3$
1-Nitro-2-naphthol
1-Nitro-naphthol-(2)
RN: 550-60-7 **MP** (°C)**:** 104
MW: 189.17 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-03	2.000E-01	20	F300	1 0 0 0 2	

2007. $C_{10}H_7NO_3$
Kynurenic acid
4-Hydroxy-chinolin-carbonsaeure-(2)
Kynurensaeure
RN: 492-27-3 **MP** (°C)**:** 282.5
MW: 189.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-02	8.920E+00	100	D041	1 0 0 0 0	
4.969E-03	9.400E-01	100	F300	1 0 0 0 1	

2008. $C_{10}H_7N_3O_3$
Orotic acid pyridine
RN: **MP** (°C)**:**
MW: 217.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.606E+01	16	N018	0 0 0 0 0	

2009. $C_{10}H_7N_3S$
Thiabendazole
2-(Thiazol-4-yl)benzimidazole
Mintezol
Apl-Luster
Mertect
Tecto
RN: 148-79-8 **MP** (°C)**:** 304.5
MW: 201.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-04	5.000E-02	25	M161	1 0 0 0 1	intrinsic

2010. $C_{10}H_8$
Naphthalene
Napthalene
Mothballs
Camphor tar
RN: 91-20-3 **MP** (°C)**:** 80.2
MW: 128.18 **BP** (°C)**:** 217.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	1.730E-02	4.99	P331	0 0 0 0 0	
1.320E-04	1.692E-02	8.20	M082	1 1 1 2 2	
1.320E-04	1.692E-02	8.20	M151	2 1 2 2 1	
1.320E-04	1.692E-02	8.24	M183	1 2 1 1 2	
1.390E-04	1.782E-02	10	J302	2 1 2 2 2	
1.580E-04	2.025E-02	9.99	P331	0 0 0 0 0	
1.500E-04	1.923E-02	11.50	M082	1 1 1 2 2	
1.500E-04	1.923E-02	11.50	M151	2 1 2 2 2	
1.502E-04	1.925E-02	11.54	M183	1 2 1 1 2	
1.570E-04	2.012E-02	12	S076	2 2 2 2 2	
1.590E-04	2.038E-02	13.40	M082	1 1 1 2 2	
1.590E-04	2.038E-02	13.40	M151	2 1 2 2 2	
1.591E-04	2.039E-02	13.44	M183	1 2 1 1 2	
1.900E-04	2.435E-02	14.99	P331	0 0 0 0 0	
1.716E-03	2.200E-01	15	F300	1 0 0 0 2	*sic*
1.716E-04	2.200E-02	15	M073	1 0 2 2 1	
1.680E-04	2.153E-02	15.10	M082	1 1 1 2 2	

(*continued*)

2010. $C_{10}H_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-04	2.153E-02	15.10	M151	2 1 2 2 2	
1.677E-04	2.150E-02	15.14	M183	1 2 1 1 2	
1.900E-04	2.435E-02	18	S076	2 2 2 2 2	
2.010E-04	2.576E-02	19.30	M082	1 1 1 2 2	
2.010E-04	2.576E-02	19.30	M151	2 1 2 2 2	
2.013E-04	2.581E-02	19.34	M183	1 2 1 1 2	
2.240E-04	2.871E-02	19.99	P331	0 0 0 0 0	
1.748E-04	2.240E-02	20	A050	1 0 1 1 1	
7.412E-04	9.500E-02	20	B318	0 0 0 0 0	EFG
3.000E-04	3.845E-02	20	E009	1 0 0 0 1	
3.000E-04	3.845E-02	20	E025	1 0 2 2 1	
1.900E-04	2.435E-02	20	H306	1 0 1 2 1	
1.272E-04	1.630E-02	20	T301	1 2 2 2 2	
2.400E-04	3.076E-02	22	A413	2 0 2 2 1	
2.645E-04	3.390E-02	22	C413	2 0 2 2 1	
1.638E-04	2.100E-02	22	N311	1 0 1 1 2	
2.255E-04	2.890E-02	22.20	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	23	P332	0 0 0 0 0	
2.341E-04	3.000E-02	23	P339	0 0 0 0 0	
2.300E-04	2.948E-02	23.40	M082	1 1 1 2 2	
2.300E-04	2.948E-02	23.40	M151	2 1 2 2 2	
2.301E-04	2.949E-02	23.44	M183	1 2 1 1 2	
2.380E-04	3.050E-02	24.50	W003	2 2 2 2 2	average of 5
2.630E-04	3.371E-02	24.99	P331	0 0 0 0 0	
2.458E-04	3.150E-02	25	A001	1 2 2 2 2	
2.350E-04	3.012E-02	25	A325	2 1 2 2 2	
2.684E-04	3.440E-02	25	B003	2 2 2 2 2	
2.465E-04	3.160E-02	25	B319	2 0 1 2 2	average of 2
2.442E-04	3.130E-02	25	D337	0 0 0 0 0	
2.715E-04	3.480E-02	25	D406	1 2 2 2 2	
2.442E-04	3.130E-02	25	E004	2 1 2 2 2	
2.620E-04	3.358E-02	25	G047	2 2 2 2 2	
2.520E-04	3.230E-02	25	J302	2 1 2 2 2	
9.750E-05	1.250E-02	25	K001	2 2 2 2 2	
2.300E-04	2.948E-02	25	K123	1 0 2 2 1	
2.497E-04	3.200E-02	25	L332	1 1 1 1 0	
2.653E-04	3.400E-02	25	M040	1 0 0 1 1	
2.550E-04	3.268E-02	25	M058	2 2 2 2 2	
2.473E-04	3.170E-02	25	M064	1 1 2 2 2	
2.472E-04	3.169E-02	25	M071	2 2 2 2 2	
3.121E-04	4.000E-02	25	M073	1 0 2 2 1	
2.620E-04	3.358E-02	25	M123	1 0 0 0 2	
2.575E-04	3.300E-02	25	M130	1 0 0 0 1	
2.390E-04	3.063E-02	25	M342	1 0 1 1 2	
2.497E-04	3.200E-02	25	O320	0 0 0 0 0	
2.575E-05	3.300E-03	25	P340	0 0 0 0 0	
2.356E-04	3.020E-02	25	R042	1 2 2 2 2	

(*continued*)

2010. $C_{10}H_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-04	2.999E-02	25	S076	2 2 2 2 2	
1.716E-04	2.200E-02	25	S227	1 2 1 1 1	
2.390E-04	3.063E-02	25	W300	2 2 2 2 2	
2.490E-04	3.192E-02	25.00	M082	1 1 1 2 2	
2.490E-04	3.192E-02	25.00	M151	2 1 2 2 2	
2.472E-04	3.169E-02	25.00	M151	2 1 1 2 2	
6.936E-04	8.890E-02	25.00	P007	2 1 2 2 2	
2.492E-04	3.194E-02	25.04	M183	1 2 1 1 2	
2.510E-04	3.217E-02	25.04	V013	2 2 2 2 2	
2.660E-04	3.409E-02	27.00	M082	1 1 1 2 2	
2.660E-04	3.409E-02	27.00	M151	2 1 2 2 2	
2.666E-04	3.417E-02	27.04	M183	1 2 1 1 2	
2.980E-04	3.820E-02	29.90	W003	2 2 2 2 2	average of 3
3.240E-04	4.153E-02	29.99	P331	0 0 0 0 0	
2.949E-04	3.780E-02	30.30	W003	2 2 2 2 2	average of 3
3.448E-04	4.420E-02	34.50	W003	2 2 2 2 2	average of 2
3.710E-04	4.755E-02	34.99	P331	0 0 0 0 0	
4.112E-04	5.270E-02	39.30	W003	2 2 2 2 2	average of 2
4.360E-04	5.588E-02	39.99	P331	0 0 0 0 0	
4.275E-04	5.480E-02	40.10	W003	2 2 2 2 2	
5.118E-04	6.560E-02	44.70	W003	2 2 2 2 2	average of 3
6.132E-04	7.860E-02	50.20	W003	2 2 2 2 2	
8.270E-04	1.060E-01	55.60	W003	2 2 2 2 2	
1.233E-03	1.580E-01	64.50	W003	2 2 2 2 2	average of 3
1.904E-03	2.440E-01	73.40	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	ns	F071	0 1 2 1 1	
2.341E-04	3.000E-02	ns	H080	0 0 0 0 1	
2.473E-04	3.170E-02	ns	H123	0 0 0 0 0	
2.473E-04	3.170E-02	ns	K304	0 0 0 0 2	
2.340E-04	2.999E-02	ns	L060	0 0 0 0 2	average
2.473E-04	3.170E-02	ns	M344	0 0 0 0 2	
2.341E-04	3.000E-02	ns	O009	0 0 0 0 0	
8.129E-04	1.042E-01	ns	R042	1 2 2 2 2	
2.341E-04	3.000E-02	rt	M161	0 0 0 0 1	
2.848E-04	3.650E-02	rt	S314	0 0 2 1 2	

2011. $C_{10}H_8BrN_3O$

Bropirimine

2-Amino-5-bromo-6-phenyl-py-rimidin-4(3H)-one

ABPP

RN: 56741-95-8 **MP** (°C)**:**

MW: 266.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.931E-05	7.800E-03	37	A346	0 0 0 0 0	EFG

2012. $C_{10}H_8BrN_3O$
Brompyrazone
Amino-4-bromo-2-phenyl-3(2H)-pyridazinone
1-Phenyl-4-amino-5-bromo-6-pyridazone
Pyridazinone, 5-amino-4-bromo-2-phenyl-
RN: 3042-84-0 **MP** (°C)**:** 223.5
MW: 266.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.516E-04	2.000E-01	20	M161	1 0 0 0 2	

2013. $C_{10}H_8ClN_3O$
Pyrazon
5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone
RN: 1698-60-8 **MP** (°C)**:** 207
MW: 221.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.353E-03	3.000E-01	20	B185	0 0 0 0 0	
1.353E-03	2.999E-01	20	B200	1 0 0 0 0	
1.353E-03	2.999E-01	20	M061	1 0 0 0 0	
1.805E-03	4.000E-01	20	M161	1 0 0 0 2	

2014. $C_{10}H_8N_2$
γ,γ′-Dipyridyl
4,4′-Bipyridyl
RN: 553-26-4 **MP** (°C)**:** 69
MW: 156.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-02	4.509E+00	25	B095	2 0 1 1 2	

2015. $C_{10}H_8N_2$
α,α′-Dipyridyl
2,2′-Dipyridyl
α,α′-Bipyridyl
2,2′-Bipyridine
2,2′-Bipyridyl
RN: 366-18-7 **MP** (°C)**:** 71.5
MW: 156.19 **BP** (°C)**:** 273

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-02	5.000E+00	20	F300	1 0 0 0 0	
4.276E-02	6.678E+00	24.99	B444	0 0 0 0 0	
3.778E-02	5.900E+00	25	B095	2 0 1 1 2	
4.094E-02	6.394E+00	25	K063	2 2 0 1 2	

2016. $C_{10}H_8N_2O_2$
4-Phenyluracil
4-Phenyl-uracil
RN: 21321-07-3 **MP** (°C)**:**
MW: 188.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.314E-02	1.000E+01	100	F300	1 0 0 0 0	

2017. $C_{10}H_8O$
1-Naphthol
α-Naphthol
RN: 90-15-3 **MP** (°C)**:** 96
MW: 144.17 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.030E-03	8.694E-01	11	K307	2 0 1 2 2	
7.700E-03	1.110E+00	20	K130	2 1 1 1 2	
7.700E-03	1.110E+00	20	K301	2 2 1 1 1	
7.700E-03	1.110E+00	20	K307	2 0 1 2 2	
6.001E-03	8.653E-01	24	H106	1 0 2 2 2	
6.007E-03	8.660E-01	24	M303	1 0 1 1 2	
3.029E-03	4.367E-01	25	L085	1 2 0 1 2	
9.430E-03	1.360E+00	30	K307	2 0 1 2 2	
1.490E-02	2.148E+00	40	K307	2 0 1 2 2	
2.150E-02	3.100E+00	50	K307	2 0 1 2 2	

2018. $C_{10}H_8O$
2-Naphthol
β-Naphthol
RN: 135-19-3 **MP** (°C)**:** 121
MW: 144.17 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	3.550E-01	6.90	M026	2 0 1 2 2	
3.378E-03	4.870E-01	13.45	M026	2 0 1 2 2	
3.473E-03	5.007E-01	15.60	M027	1 0 0 2 2	
3.646E-03	5.257E-01	16.20	M027	1 0 0 2 2	
3.891E-03	5.610E-01	17.70	M026	2 0 1 2 2	
4.450E-03	6.416E-01	20	K130	2 1 1 1 2	
4.500E-03	6.488E-01	20	K301	2 2 1 1 1	
4.450E-03	6.416E-01	20	K308	1 0 0 1 2	
5.800E-03	8.362E-01	20	M122	2 0 2 2 2	
4.945E-03	7.130E-01	21.50	M026	2 0 1 2 2	
4.713E-03	6.795E-01	23.20	M027	1 0 0 2 2	
3.954E-03	5.700E-01	25	F300	1 0 0 0 2	

(*continued*)

2018. $C_{10}H_8O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.240E-03	7.555E-01	25	K040	1 0 2 1 2	
5.356E-03	7.722E-01	25	L085	1 2 0 1 2	
6.929E-03	9.990E-01	25	R041	0 0 0 0 0	
6.076E-03	8.760E-01	29.50	M026	2 0 1 2 2	
6.431E-03	9.271E-01	31.30	M027	1 0 0 2 2	
6.832E-03	9.850E-01	33.30	M026	2 0 1 2 2	
9.045E-03	1.304E+00	38.70	M026	2 0 1 2 2	
1.116E-02	1.609E+00	44.50	M026	2 0 1 2 2	
1.388E-02	2.001E+00	49.50	M026	2 0 1 2 2	
1.706E-02	2.460E+00	55.20	M026	2 0 1 2 2	
2.104E-02	3.034E+00	60.00	M026	2 0 1 2 2	
2.928E-02	4.222E+00	68.10	M026	2 0 1 2 2	
3.810E-02	5.493E+00	75.00	M026	2 0 1 2 2	
4.670E-02	6.733E+00	80	K308	1 0 0 1 2	
5.129E-03	7.394E-01	ns	R427	0 0 0 0 0	

2019. $C_{10}H_8O_2$
2,3-Dihydroxynaphthalene
2,3-Dihydroxy-naphthalin
RN: 92-44-4 **MP** (°C)**:** 162
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-03	2.931E-01	20	M122	2 0 2 2 2	

2020. $C_{10}H_8O_2$
2,6-Dihydroxynaphthalene
2,6-Dihydroxy-naphthalin
RN: 581-43-1 **MP** (°C)**:**
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-03	1.000E+00	14	F300	1 0 0 0 0	

2021. $C_{10}H_9ClN_4O_2S$
2-Sulfanilamido-5-chloropyrimidine
Benzenesulfonamide, 4-amino-*N*-(5-chloro-2-pyrimidinyl)-
RN: 4482-46-6 **MP** (°C)**:**
MW: 284.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.322E-05	1.800E-02	37	R046	1 2 1 1 1	

2022. $C_{10}H_9ClN_4O_2S$
5-Sulfanilamido-2-chloropyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-chloro-5-pyrimidinyl)-
RN: 17103-49-0 **MP** (°C)**:**
MW: 284.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.127E-03	3.210E-01	37	R046	1 2 1 1 1	

2023. $C_{10}H_9Cl_2NO$
Acrylanilide, 3′,4′-dichloro-2-methyl-
Dicryl
RN: 2164-09-2 **MP** (°C)**:** 127–128
MW: 230.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-05	8.000E-03	ns	B185	0 0 0 0 0	

2024. $C_{10}H_9Cl_3O_3$
2,4,5-Trichlorophenoxy-γ-butyric acid
2,4,5-TB
4-(2,4,5-Trichlorophenoxy)butyric acid
4-(2,4,5-TB)
RN: 93-80-1 **MP** (°C)**:** 114.5
MW: 283.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-04	4.200E-02	25	B164	1 0 1 1 1	
1.481E-04	4.200E-02	ns	B185	0 0 0 0 0	

2025. $C_{10}H_9Cl_3O_3$
2,4-Dichlorophenoxyacetic acid β-monochloroethyl ester
Ethanol, 2-chloro-, (2,4-dichlorophenoxy)acetate
RN: 19810-30-1 **MP** (°C)**:**
MW: 283.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-04	5.415E-02	ns	M120	0 0 1 1 2	

2026. $C_{10}H_9Cl_4NO_2S$
Captafol
cis-3α,4,7,7α-Tetrahydro-2-(1,1,2,2-tetrachloroethyl)thio-1H-isoindole-1,3(2H)-dione
Crisfolatan
Difolatan
Folcid
RN: 2939-80-2 **MP** (°C)**:** 160.5
MW: 349.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-06	1.422E-03	20	B179	0 0 0 0 0	
4.011E-06	1.400E-03	ns	M161	0 0 0 0 1	

2027. $C_{10}H_9Cl_4O_4P$
Gardona
2-Chloro-1-(2,4,5-trichlorophenyl)vinyldimethylphosphate
RN: 22248-79-9 **MP** (°C)**:** 97.5
MW: 365.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M061	1 0 0 0 1	

2028. $C_{10}H_9Cl_4O_4P$
Tetrachlorvinphos
2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate
Rabon
Gardona
SD 8447
Stirofos
RN: 961-11-5 **MP** (°C)**:** 96
MW: 365.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M161	1 0 0 0 1	

2029. $C_{10}H_9N$
3-Methyl-isoquinoline
Isoquinoline, 3-methyl-
RN: 1125-80-0 **MP** (°C)**:**
MW: 143.19 **BP** (°C)**:** 519.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-03	9.190E-01	20	A050	1 0 1 1 2	

2030. $C_{10}H_9N$
2-Naphthylamine
Naphthylamine-(2)
β-Naphthylamin
β-Naphthylamine
RN: 91-59-8 **MP** (°C)**:** 113
MW: 143.19 **BP** (°C)**:** 306.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.320E-03	1.890E-01	rt	N015	0 0 2 2 2	

2031. $C_{10}H_9N$
1-Naphthylamine
1-Aminonaphthalene
α-Naphthoylamine
α-Naphthylamin
α-Naphthylamine
RN: 134-32-7 **MP** (°C)**:** 50
MW: 143.19 **BP** (°C)**:** 300.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	1.700E+00	20	F300	1 0 0 0 1	
3.600E-04	5.155E-02	ns	L060	0 0 0 0 1	average

2032. $C_{10}H_9NO$
8-Hydroxyquinaldine
2-Methyl 8-quinolinol
RN: 826-81-3 **MP** (°C)**:** 72.5
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E+03	3.916E+05	25.2	P024	2 2 1 1 2	
2.670E+03	4.250E+05	30.3	P024	2 2 1 1 2	

2033. $C_{10}H_9NO$
4-Hydroxy-2-methylquinoline
4-Hydroxy-2-methyl-chinolin
RN: 607-67-0 **MP** (°C)**:** 234
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.282E-02	1.000E+01	20	F300	1 0 0 0 1	
5.936E-01	9.450E+01	100	F300	1 0 0 0 2	

2034. $C_{10}H_9NO_2S$
Ethyl *m*-isothiocyanobenzoate
Ethyl 3-isothiocyanobenzoate
RN: 3137-84-6 **MP** (°C)**:**
MW: 207.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	5.181E-02	25	K032	2 2 0 1 2	

2035. $C_{10}H_9NO_2S$
Ethyl 4-isothiocyanatobenzoate
4-Carbethoxyphenylisothiocyanate
Ethyl *p*-isothiocyanatobenzoate
RN: 1205-06-7 **MP** (°C)**:**
MW: 207.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	1.865E-02	25	D019	1 1 1 1 1	

2036. $C_{10}H_9NO_3S$
Badische acid
2-Naphthylamine-8-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(8)
RN: 86-60-2 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-03	6.000E-01	20	F300	1 0 0 0 2	

2037. $C_{10}H_9NO_3S$
2-Naphthylamine-1-sulfonic acid
α-Naphthylamine-*o*-monosulfonic acid
RN: 81-16-3 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	2.394E+00	0	D077	1 0 0 1 1	
1.429E-02	3.190E+00	10	D077	1 0 0 1 1	
1.829E-02	4.083E+00	20	D077	1 0 0 1 1	
2.317E-02	5.173E+00	30	D077	1 0 0 1 1	
2.893E-02	6.458E+00	40	D077	1 0 0 1 1	
3.555E-02	7.937E+00	50	D077	1 0 0 1 1	
4.435E-02	9.901E+00	60	D077	1 0 0 1 2	
6.010E-02	1.342E+01	70	D077	1 0 0 1 2	
7.834E-02	1.749E+01	80	D077	1 0 0 1 2	
1.028E-01	2.296E+01	90	D077	1 0 0 1 2	
1.347E-01	3.007E+01	100	D077	1 0 0 1 2	

2038. $C_{10}H_9NO_3S$
1-Naphthylamine-8-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(8)
Peri acid
RN: 82-75-7 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	21	F300	1 0 0 0 0	
1.971E-02	4.400E+00	100	F300	1 0 0 0 1	

2039. $C_{10}H_9NO_3S$
1-Naphthylamine-5-sulfonic acid
Laurent's acid
Naphthylamin-(1)-sulfosaeure-(5)
RN: 84-89-9 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	20	F300	1 0 0 0 2	

2040. $C_{10}H_9NO_3S$
1-Naphthylamine-4-sulfonic acid
4-Amino-1-naphthalenesulfonic acid
Naphthionic acid
Naphthylamin-(1)-sulfosaeure-(4)
Pirias acid
RN: 84-86-6 **MP** (°C)**:** 000
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-03	2.699E-01	0	D077	1 0 0 1 1	
1.299E-03	2.899E-01	10	D077	1 0 0 1 1	
1.388E-03	3.099E-01	20	D077	1 0 0 1 1	
1.344E-03	3.000E-01	20	F300	1 0 0 0 0	
1.657E-03	3.699E-01	30	D077	1 0 0 1 1	
2.149E-03	4.798E-01	40	D077	1 0 0 1 1	
2.641E-03	5.897E-01	50	D077	1 0 0 1 1	
3.357E-03	7.494E-01	60	D077	1 0 0 1 1	
4.341E-03	9.691E-01	70	D077	1 0 0 1 1	
5.815E-03	1.298E+00	80	D077	1 0 0 1 2	
7.825E-03	1.747E+00	90	D077	1 0 0 1 2	
1.021E-03	2.279E-01	100	D077	1 0 0 1 2	
1.075E-02	2.400E+00	100	F300	1 0 0 0 1	

2041. $C_{10}H_9NO_3S$
1,6-Cleve's acid
1-Naphthylamine-6-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(6)
RN: 119-79-9 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	16	F300	1 0 0 0 2	

2042. $C_{10}H_9NO_3S$
Cassella's acid F
2-Naphthylamine-7-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(7)
RN: 494-44-0 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	20	F300	1 0 0 0 1	
1.389E-02	3.100E+00	100	F300	1 0 0 0 1	

2043. $C_{10}H_9NO_3S$
Bronner's acid
2-Naphthylamine-6-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(6)
RN: 93-00-5 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.375E-04	1.200E-01	20	F300	1 0 0 0 1	
7.615E-03	1.700E+00	100	F300	1 0 0 0 1	

2044. $C_{10}H_9NO_3S$
1-Naphthylamine-2-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(2)
RN: 81-06-1 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	4.100E+00	20	F300	1 0 0 0 1	
1.402E-01	3.130E+01	100	F300	1 0 0 0 2	

2045. $C_{10}H_9NO_3S$
2-Naphthylamine-5-sulfonic acid
Dahl's acid
Naphthylamin-(2)-sulfosaeure-(5)
RN: 81-05-0 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	3.300E-01	20	F300	1 0 0 0 2	

2046. $C_{10}H_9NO_4S$
7-Amino-1-naphthol-3-sulfonic acid
7-Amino-naphtol-(1)-sulfosaeure-(3)
RN: 90-51-7 **MP** (°C)**:**
MW: 239.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-02	4.500E+00	h	F300	0 0 0 0 1	

2047. $C_{10}H_9NO_9S_3$
1-Naphthylamine-2,4,7-trisulfonic acid
1,3,6-Naphthalenetrisulfonic acid, 4-amino-
RN: 61986-93-4 **MP** (°C)**:**
MW: 383.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.799E-01	1.840E+02	20	F054	1 2 1 1 2	
8.216E-01	3.150E+02	80	F054	1 2 1 1 2	

2048. $C_{10}H_9N_3O_3S$
1-Sulfanilyl-3-methyl-5-pyrazolone
RN: **MP** (°C)**:**
MW: 251.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-03	4.590E-01	37	R045	1 2 1 1 2	

2049. $C_{10}H_9N_4O_5$
Picrolonic acid
Pikrolonsaeure
RN: 550-74-3 **MP** (°C)**:** 116
MW: 265.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.394E-02	9.000E+00	17	F300	1 0 0 0 0	
3.582E-02	9.500E+00	100	F300	1 0 0 0 1	

2050. $C_{10}H_{10}Fe$
Ferrocene
bis-Cyclopentadienyliron
Ferrotsen
Iron bis(cyclopentadiene)
RN: 102-54-5 **MP** (°C)**:**
MW: 186.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-05	6.304E-03	25	B335	1 2 0 0 1	

2051. $C_{10}H_{10}BrNO_3S$
4-Thiazolidinecarboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-
RN: 256235-53-7 **MP** (°C)**:**
MW: 304.17 **BP** (°C)**:** 451.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.650E-01	21	B414	1 0 0 1 1	fast decomposition

2052. $C_{10}H_{10}BrNO_4$
5-Bromo-2-*p*-phenyl-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-5-nitro-2-phenyl-
1,3-Dioxane, 5-bromo-5-nitro-2-phenyl-
RN: 58522-87-5 **MP** (°C)**:** 82–84
MW: 288.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	4.598E-01	25	L013	1 0 2 1 2	

2053. $C_{10}H_{10}BrNO_5$
5-Bromo-2-*p*-phenol-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-5-nitro-2-phenol-
RN: 60766-61-2 **MP** (°C)**:** 142–144
MW: 304.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	4.298E-01	25	L013	1 0 2 1 2	

2054. $C_{10}H_{10}ClNO_2S$
4-Thiazolidinecarboxylic acid, 2-(4-chlorophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*p*-chlorophenyl)-
Thiazolidine-4-carboxylic acid, (2-(4-chlorophenyl)-
RN: 34491-29-7 **MP** (C)**:** 156-185 (°decomp)
MW: 243.71 **BP** (°C)**:** 458.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-03	1.438E+00	21	B414	1 0 0 1 1	fast decomposition

2055. $C_{10}H_{10}ClNO_2S$
4-Thiazolidinecarboxylic acid, 2-(2-chlorophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*o*-chlorophenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-chlorophenyl)-
RN: 72678-81-0 **MP** (°C)**:** 145–147
MW: 243.71 **BP** (°C)**:** 439.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.118E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2056. $C_{10}H_{10}ClNO_3$
Chloroacetyl acetaminophen
Acetic acid, chloro-, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, chloroacetate (ester)
RN: 17321-63-0 **MP** (°C)**:** 184.5–185
MW: 227.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	2.800E-01	37	D029	0 0 0 0 0	

2057. $C_{10}H_{10}Cl_2F_2N_2OS$
3-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-1,1-dimethylurea
N-[3-Chloro-4-(chlorodifluoromethylthiol)phenyl]-*N′,N′*-dimethylurea
N-(3-Chloro-4-difluorochloromethylthiophenyl)-*N′,N′*-dimethylurea
Thiochlormethyl
N-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-*N′,N′*-dimethylurea
RN: 33439-45-1 **MP** (°C)**:** 113.5
MW: 315.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.159E-01	6.803E+01	20	M161	1 0 0 0 1	

2058. $C_{10}H_{10}Cl_2O_2$
Chlorfenprop-methyl
Methyl 2-chloro-3-(*p*-chlorophenyl)propionate
Methyl α-*p*-dichlorohydrocinnamate
Bidisin
Fatex
RN: 14437-17-3 **MP** (°C)**:**
MW: 233.10 **BP** (°C)**:** 111.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.716E-04	4.000E-02	20	M161	1 0 0 0 1	

2059. $C_{10}H_{10}Cl_2O_3$
4-(2,4-Dichlorophenoxy)propionic acid
2,4-DB
RN: 94-82-6 **MP** (°C)**:** 118
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	6.700E-02	25	B164	1 0 1 1 1	
1.847E-04	4.600E-02	25	M161	1 0 0 0 1	
2.128E-04	5.300E-02	ns	B185	0 0 0 0 0	
1.847E-04	4.600E-02	ns	L024	1 0 0 0 1	
2.128E-04	5.300E-02	rt	M061	0 0 0 0 1	

2060. $C_{10}H_{10}Cl_2O_3$
Ethyl (2,4-dichlorophenoxy)acetate
2,4-Dichlorophenoxyacetic acid ethyl ester
RN: 533-23-3 **MP** (°C)**:**
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.529E-04	6.300E-02	ns	M120	0 0 1 1 2	

2061. $C_{10}H_{10}Cl_8$
Toxaphene
Camphechlor
Campheclor
PhenAcide
Toxakil
Chlorinated champhene
RN: 8001-35-2 **MP** (°C)**:** 65
MW: 413.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-06	5.500E-04	20	M336	2 0 2 2 2	
9.666E-07	4.000E-04	25	C100	1 0 2 1 0	
1.208E-06	5.000E-04	25	P085	0 0 0 0 0	
1.788E-06	7.400E-04	25	W025	1 0 2 2 2	
1.450E-06	6.000E-04	ns	M110	0 0 0 0 0	EFG
1.329E-06	5.500E-04	ns	V414	0 0 0 0 0	
7.250E-06	3.000E-03	rt	M161	0 0 0 0 0	

2062. $C_{10}H_{10}N_2O_4S$
4-Thiazolidinecarboxylic acid, 2-(3-nitrophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*m*-nitrophenyl)-
RN: 69570-81-6 **MP** (°C)**:** 151–153
MW: 254.27 **BP** (°C)**:** 500.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.348E+00	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2063. $C_{10}H_{10}N_4O$
Metamitron
3-Methyl-4-amino-6-phenyl-1,2,4-triazin-5(4H)-one
4-Amino-3-methyl-6-phenyl-1,2,4-triazin-5-one
Goltix
RN: 41394-05-2 **MP** (°C)**:** 166.6
MW: 202.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.901E-03	1.800E+00	20	M161	1 0 0 0 1	

2064. $C_{10}H_{10}N_4O_2S$

Sulfadiazine
Sulphadiazine
*N*1-(2-Pyrimidinyl)-sulfanilamide
Debenal

RN: 68-35-9 **MP** (°C)**:** 254
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-04	5.907E-02	20	C006	1 2 1 1 2	
1.814E-04	4.540E-02	20	E003	2 2 1 1 2	
5.993E-04	1.500E-01	20	F073	1 2 2 2 2	
2.917E-04	7.299E-02	20	L058	1 0 1 1 1	
3.077E-04	7.700E-02	25	C102	2 0 2 2 2	
2.637E-03	6.600E-01	25	K048	1 2 2 1 1	pH 1.26
2.682E-04	6.713E-02	25	M440	0 0 0 0 0	
3.036E-04	7.599E-02	30	E003	2 2 1 1 2	
3.640E-04	9.110E-02	30	H018	0 0 0 0 0	
3.200E-04	8.009E-02	30	L069	1 0 1 1 0	EFG
7.192E-04	1.800E-01	35	H114	1 0 0 0 1	
5.074E-04	1.270E-01	37	C102	2 0 2 2 2	
4.914E-04	1.230E-01	37	F072	1 0 0 0 2	
4.794E-04	1.200E-01	37	F075	1 0 2 2 2	
5.114E-04	1.280E-01	37	K091	1 0 0 0 2	
5.194E-04	1.300E-01	37	L091	1 0 0 0 1	pH 5.5
7.192E-04	1.800E-01	37	M057	1 0 0 0 2	pH 5.5
8.790E-04	2.200E-01	37	R044	0 0 0 0 0	EFG, intrinsic
4.914E-04	1.230E-01	37	R045	1 2 1 1 1	
6.712E-04	1.680E-01	37	S192	1 0 1 1 2	pH 6.0
5.074E-04	1.270E-01	37	W016	2 0 1 1 2	
4.914E-04	1.230E-01	37	W053	1 0 0 0 2	
3.956E-04	9.900E-02	38	K006	1 0 0 0 1	
5.154E-04	1.290E-01	40	E003	2 2 1 1 2	
5.194E-04	1.300E-01	ns	G083	0 0 0 0 1	pH 5.5
3.196E-04	8.000E-02	ns	K444	0 0 0 0 0	
3.981E-04	9.964E-02	ns	R427	0 0 0 0 0	

2065. $C_{10}H_{10}N_4O_2S$

Sulfapyrazine
Sulphapyrazine

RN: 116-44-9 **MP** (°C)**:** 255
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2066. $C_{10}H_{10}N_4O_2S$
5-Sulfanilamidopyrimidine
5-Sulfapyrimidine
Sulfanilamide, *N*1-5-pyrimidinyl-
RN: 17103-48-9 **MP** (°C)**:**
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.916E-04	9.800E-02	37	R046	1 2 1 1 1	

2067. $C_{10}H_{10}N_4O_2S$
4-Sulfanilamidopyrimidine
4-Sulfapyrimidine
Sulfanilamide, *N*1-4-pyrimidinyl-
RN: 599-82-6 **MP** (°C)**:**
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.414E-02	3.540E+00	37	R045	1 2 1 1 2	

2068. $C_{10}H_{10}N_4O_4S$
5-Sulfanilamidouracil
Benzenesulfonamide, 4-amino-*N*-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)-
RN: 6912-98-7 **MP** (°C)**:**
MW: 282.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.722E-03	4.860E-01	37	R045	1 2 1 1 0	

2069. $C_{10}H_{10}O$
Benzalacetone
4-Phenyl-3-buten-2-one
Methyl styryl ketone
RN: 122-57-6 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-03	1.398E+00	25	R070	0 0 0 0 0	

2070. $C_{10}H_{10}O_2$
p-Acetylacetophenone
Ethanone, 1,1′-(1,4-phenylene)*bis*-
RN: 1009-61-6 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-05	6.309E-03	25	C316	0 0 0 0 0	0.1M NaCl

2071. $C_{10}H_{10}O_2$
Methyl cinnamate
2-Propenoic acid
3-Phenyl-, methyl ester
RN: 103-26-4 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.055E-01	25	R070	0 0 0 0 0	

2072. $C_{10}H_{10}O_2$
trans-α-Methyl-cinnamic acid
α-Methyl-*trans*-zimtsaeure
RN: 1895-97-2 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.399E-03	1.200E+00	h	F300	0 0 0 0 1	

2073. $C_{10}H_{10}O_4$
Dimethyl *o*-phthalate
RN: **MP** (°C)**:** 5.5 C
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.802E-02	3.500E+00	25	S417	0 0 0 0 0	

2074. $C_{10}H_{10}O_4$
Ferulic acid
3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid
4-Hydroxy-3-methoxycinnamic acid
RN: 1135-24-6 **MP** (°C)**:** 169 C
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.935E-03	5.700E-01	15	M461	0 0 0 0 0	
4.017E-03	7.800E-01	25	M461	0 0 0 0 0	
4.738E-03	9.200E-01	30	M461	0 0 0 0 0	
9.063E-03	1.760E+00	40	M461	0 0 0 0 0	
1.128E-02	2.190E+00	50	M461	0 0 0 0 0	

2075. $C_{10}H_{10}O_4$
Acetyl-*r*-mandelic acid
(R)(–)*O*-Acetylmandelic acid
[R]-[–]-α-(Acetoxy)phenylacetic acid
O-Acetylmandelic acid
RN: 5438-68-6 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.919E-02	5.668E+00	0	A043	1 2 1 1 1	
2.919E-02	5.668E+00	0	L035	1 2 2 1 1	
3.478E-02	6.754E+00	10	A043	1 2 1 1 1	
3.478E-02	6.754E+00	10	L035	1 2 2 1 1	
3.884E-02	7.543E+00	15	A043	1 2 1 1 1	
3.884E-02	7.543E+00	15	L035	1 2 2 1 1	
4.897E-02	9.509E+00	20	A043	1 2 1 1 1	
4.897E-02	9.509E+00	20	L035	1 2 2 1 1	
5.804E-02	1.127E+01	25	A043	1 2 1 1 2	
5.804E-02	1.127E+01	25	L035	1 2 2 1 2	
7.060E-02	1.371E+01	30	A043	1 2 1 1 2	
7.060E-02	1.371E+01	30	L035	1 2 2 1 2	
1.005E-01	1.951E+01	35	A043	1 2 1 1 2	
1.587E-01	3.082E+01	40	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	L035	1 2 2 1 2	
6.125E-01	1.189E+02	50	A043	1 2 1 1 2	
6.125E-01	1.189E+02	50	L035	1 2 2 1 2	

2076. $C_{10}H_{10}O_4$
Dimethyl phthalate
1,2-Benzenedicarboxylic acid, dimethyl ester
Fermine
Unimoll DM
Mipax
Palatinol M
RN: 131-11-3 **MP** (°C)**:** 5.5
MW: 194.19 **BP** (°C)**:** 283.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-02	4.292E+00	20	L300	2 1 0 2 2	
4.087E-02	7.937E+00	20.00	D343	0 0 0 0 0	
2.317E-01	4.500E+01	25	F067	1 0 2 2 2	*sic*
2.307E-02	4.480E+00	c	F070	1 0 0 0 0	
1.566E-02	3.041E+00	ns	F014	0 0 0 0 2	
2.052E-02	3.984E+00	ns	H069	0 0 1 1 1	
2.214E-02	4.300E+00	rt	M161	0 0 0 0 1	

2077. $C_{10}H_{10}O_4$
Meconin
Mekonin
RN: 569-31-3 **MP** (°C)**:** 102
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.287E-02	2.500E+00	25	F300	1 0 0 0 0	
2.420E-02	4.700E+00	100	F300	1 0 0 0 1	

2078. $C_{10}H_{10}O_4$
Acetylsalicylic acid, methyl ester
Methyl 2-acetoxybenzoate
Benzoic acid, 2-(acetyloxy)-, methyl ester
RN: 580-02-9 **MP** (°C)**:** 48
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-02	2.810E+00	21	N335	0 0 0 0 0	
1.679E-02	3.260E+00	37	G430	0 0 0 0 0	pH 4.5

2079. $C_{10}H_{10}O_4$
Terephthalate acid dimethyl ester
Terephthalsaeure-dimethyl ester
1,4-Benzenedicarboxylic acid dimethyl ester
Terephthalic acid
Dimethyl terephthalate
Dimethyl 1,4-Benzenedicarboxylate
RN: 120-61-6 **MP** (°C)**:** 140
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-04	3.282E-02	25	C316	0 0 0 0 0	0.1M NaCl
1.540E-02	2.991E+00	h	F070	1 0 0 0 1	

2080. $C_{10}H_{10}O_5$
Opianic acid
Opiansaeure
RN: 519-05-1 **MP** (°C)**:** 150
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.189E-02	2.500E+00	20	F300	1 0 0 0 1	
8.088E-02	1.700E+01	h	F300	0 0 0 0 1	

2081. $C_{10}H_{11}ClO_3$
Mecoprop
2-(4-Chloro-2-methylphenoxy)propionic acid
2-(2-Methyl-4-chlorophenoxy)propionic acid
2-(MCPP)
RN: 93-65-2 **MP** (°C)**:** 93
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-03	6.200E-01	20	B185	0 0 0 0 0	
2.795E-03	6.000E-01	20	B200	1 0 0 0 2	
2.887E-03	6.196E-01	20	M061	1 0 0 0 1	
2.888E-03	6.200E-01	20	M161	1 0 0 0 2	
4.170E-03	8.950E-01	25	B164	1 0 1 1 2	
4.170E-03	8.950E-01	25	B185	0 0 0 0 0	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.050E-04	4.400E-02	ns	B185	0 0 0 0 0	
2.888E-03	6.200E-01	ns	L024	1 0 0 0 2	
3.802E-03	8.161E-01	ns	R427	0 0 0 0 0	

2082. $C_{10}H_{11}ClO_3$
4-(4-Chlorophenoxy)butyric acid
4-(4-CPB)
RN: 3547-07-7 **MP** (°C)**:**
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.125E-04	1.100E-01	25	B164	1 0 1 1 2	

2083. $C_{10}H_{11}Cl_3O_2$
2,3,6-Trichlorobenzyloxypropanol
1-Propanol, 3-[(2,3,6-trichlorobenzyl)oxy]-
RN: 1591-82-8 **MP** (°C)**:**
MW: 269.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.708E-04	7.300E-02	25	B185	0 0 0 0 0	
2.708E-04	7.300E-02	25	B200	1 0 0 0 1	

2084. $C_{10}H_{11}FN_2O_6$
1,3-bis(Acetoxymethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1,3-bis(Acetoxymethyl)-5-fluorouracil
RN: 66542-48-1 **MP** (°C)**:** 105–106
MW: 274.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.568E-02	4.300E+00	22	B321	0 0 0 0 0	pH 4.0

2085. $C_{10}H_{11}F_3N_2O$
Fluometuron
1,1-Dimethyl-3-(α,α,α-trifluoro-*m*-tolyl)urea
RN: 2164-17-2 **MP** (°C)**:** 163
MW: 232.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.061E-01	20	B179	0 0 0 0 0	
4.522E-04	1.050E-01	20	M161	1 0 0 0 2	
3.661E-04	8.500E-02	24	C105	2 1 2 2 2	
3.876E-04	9.000E-02	25	B200	1 0 0 0 1	
3.876E-04	9.000E-02	25	G036	1 0 0 0 1	
3.876E-04	9.000E-02	25	M061	1 0 0 0 1	

2086. $C_{10}H_{11}F_3N_2O_3S$
Fluoridamid
Acetamide, *N*-{4-methyl-3-{{(trifluoromethyl)sulfonyl}amino}phenyl}-
Sustar
MBR6033
RN: 47000-92-0 **MP** (°C)**:** 182–184
MW: 296.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.388E-04	1.300E-01	22	G307	0 0 0 0 0	

2087. $C_{10}H_{11}NO$
N-Methylcinnamide
2-Propenamide, *N*-methyl-3-phenyl-
RN: 2757-10-0 **MP** (°C)**:**
MW: 161.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-02	2.112E+00	ns	H350	0 0 0 0 0	

2088. $C_{10}H_{11}NOS$
m-Isopropoxyphenyl isothiocyanate
3-Isopropoxyphenyl isothiocyanate
RN: 3528-90-3 **MP** (°C)**:**
MW: 193.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	9.084E-02	25	K032	2 2 0 1 2	

2089. $C_{10}H_{11}NO_2S$
2-Phenylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-phenyl-
RN: 42607-21-6 **MP** (°C)**:** 166–168
MW: 209.27 **BP** (°C)**:** 433.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	9.417E-01	21	B414	1 0 0 1 1	partial decomposition

2090. $C_{10}H_{11}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-methyl-
RN: 106231-50-9 **MP** (°C)**:** 111
MW: 193.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-02	3.700E+00	22	B427	1 0 0 1 1	in 0.01M HCl
1.915E-02	3.700E+00	22	N317	1 1 2 1 2	

2091. $C_{10}H_{11}NO_3$
p-Acetoxy-acetanilide
p-Acetoxyacetanilide
Acetaminophen acetate
Acetyl acetaminophen
RN: 2623-33-8 **MP** (°C)**:** 153
MW: 193.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.656E-03	3.200E-01	25	B010	1 1 1 1 0	
1.237E-02	2.390E+00	25	E016	1 1 1 1 2	
1.139E-02	2.200E+00	25	M333	1 1 0 0 2	
1.760E-02	3.400E+00	37	D029	0 0 0 0 0	

2092. $C_{10}H_{11}NO_3S$
4-Thiazolidinecarboxylic acid, 2-(4-hydroxyphenyl)-
4-Thiazolidinecarboxylic acid, 2-(*p*-hydroxyphenyl)-
RN: 69588-11-0 **MP** (°C)**:**
MW: 225.27 **BP** (°C)**:** 507.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-03	1.577E+00	21	B414	1 0 0 1 1	fast decomposition

2093. $C_{10}H_{11}NO_3S$
2-(2-Hydroxyphenyl)-4-thiazolidinecarboxylic acid
4-Thiazolidinecarboxylic acid, 2-(2-hydroxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-hydroxyphenyl)
RN: 72678-82-1 **MP** (°C)**:**
MW: 225.27 **BP** (°C)**:** 418.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	4.731E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2094. $C_{10}H_{11}NO_4$
Methyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl methyl ester
Acetanilide, 4′-hydroxy-, methyl carbonate (ester)
RN: 17321-62-9 **MP** (°C)**:** 115.5–116.5
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.868E-02	6.000E+00	37	D029	0 0 0 0 0	

2095. $C_{10}H_{11}NO_4$
O-(Acetoxymethyl) salicylamide
2-[(Acetyloxy)methoxy]-benzamide
Benzamide, 2-[(acetyloxy)methoxy]-
O-Acetoxymethyl methyl salicylamide
RN: 102273-25-6 **MP** (°C)**:** 92.5
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.39E-02	>5.00E+00	23	B328	1 2 2 1 1	pH 4
2.390E-02	5.000E+00	23	B328	0 0 0 0 0	

2096. $C_{10}H_{11}NO_4$
Carbobenzoxyglycine
N-Carbobenzyloxyglycine
N-CBZ-glycine
Benzyloxycarbonyl glycine
RN: 1138-80-3 **MP** (°C)**:**
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.180E-02	4.560E+00	25.1	N026	0 0 0 0 0	
2.170E-02	4.539E+00	25.1	N027	1 1 2 2 2	

2097. $C_{10}H_{11}NO_5$
Acido D-feniltartrammico tartranilico
RN: **MP** (°C)**:** 194
MW: 225.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	2.774E+01	17.40	C070	1 2 2 1 2	

2098. $C_{10}H_{11}NO_6$
Acido *p*-ossifeniltartrammico
RN: **MP** (°C)**:** 218
MW: 241.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-01	4.045E+01	14	C071	1 2 0 1 2	

2099. $C_{10}H_{11}N_3OS$
Methabenzthiazuron
N-2-Benzothiazolyl-*N,N′*-dimethylurea
1,3-Dimethyl-3-(2-benzothiazolyl)urea
Methyl-*N′*-methyl-*N′*-(2-benzothiazolyl)urea
Tribunil
Preparation 5633
RN: 18691-97-9 **MP** (°C)**:** 119.5
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-04	5.900E-02	20	M161	1 0 0 0 1	

2100. $C_{10}H_{11}N_3O_2S_2$
Methyl sulfathiazole
Sulfathiazol methyle
RN: 15251-46-4 **MP** (°C)**:**
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.653E-04	2.600E-01	37	D084	1 0 1 0 1	

2101. $C_{10}H_{11}N_3O_2S$
Sulfapyrrole
RN: **MP** (°C)**:**
MW: 237.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.023E-02	4.800E+00	20	F073	1 2 2 2 2	

2102. $C_{10}H_{11}N_3O_2S_2$
Sulfamethylthiazole
4-Methyl-2-sulfanilamidothiazole
2-(*p*-Aminobenzenesulfonamido)-4-methylthiazole
2-Sulfanilamido-4-methylthiazole
Aseptil 2
Ciba 3753
RN: 515-59-3 **MP** (°C)**:** 239
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.084E-04	1.100E-01	20	F073	1 2 2 2 2	
4.084E-04	1.100E-01	20	F074	1 0 0 0 2	

2103. $C_{10}H_{11}N_3O_2S_2$
*N*1-Methyl-*N*1-2-thiazolyl-sulfanilamide
*N*1-Methylsulfathiazole
RN: 51203-19-1 **MP** (°C)**:**
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	3.097E-01	37	K095	2 0 0 0 2	intrinsic

2104. $C_{10}H_{11}N_3O_3$
α-Semicarbazono-*p*-tolyl acetate
RN: **MP** (°C)**:**
MW: 221.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	3.097E-01	25	A066	1 0 1 1 1	

2105. $C_{10}H_{11}N_3O_3S$
Sulfamethoxazole
4-Amino-*N*-(5-methyl-3-isoxazolyl)benzenesulfonamide
Cotrimoxazole
Septra
Bactrim
Cotrim
RN: 723-46-6 **MP** (°C)**:** 167
MW: 253.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.810E-01	25	D308	0 0 0 0 0	pH 3.22
1.730E-03	4.383E-01	25	F415	0 0 0 0 0	Average

(*continued*)

2105. $C_{10}H_{11}N_3O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-03	3.723E-01	25	M440	0 0 0 0 0	
1.974E-03	5.000E-01	25	R025	0 0 0 0 0	
1.488E-03	3.770E-01	32	D308	0 0 0 0 0	pH 4.0
1.824E-03	4.620E-01	37	D308	0 0 0 0 0	pH 3.43
2.408E-03	6.100E-01	37	H120	1 1 1 1 1	normal saline
2.480E-03	6.281E-01	37	K095	2 0 0 0 2	intrinsic
5.527E-03	1.400E+00	37	M321	1 0 0 0 2	intrinsic
1.540E-03	3.900E-01	amb	L434	0 0 0 0 0	
1.540E-03	3.900E-01	amb	L437	0 0 0 0 0	
3.948E-05	1.000E-02	ns	K444	0 0 0 0 0	

2106. $C_{10}H_{11}N_5O_2S$

5-Sulfanilamido-2-aminopyrimidine

Benzenesulfonamide, 4-amino-*N*-(2-amino-5-pyrimidinyl)-

RN: 71119-38-5 **MP** (°C)**:**

MW: 265.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-04	8.300E-02	37	R046	1 2 1 1 1	

2107. $C_{10}H_{12}$

Tetralin

1,2,3,4-Tetrahydronaphthalene

RN: 119-64-2 **MP** (°C)**:** –31.0

MW: 132.21 **BP** (°C)**:** 207.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E-04	4.500E-02	20	B356	0 0 0 0 0	
3.532E-04	4.670E-02	28	B348	2 1 2 2 2	
1.513E-03	2.000E-01	150	J023	1 1 2 2 0	
3.026E-03	4.000E-01	200	J023	1 1 2 2 0	
3.026E-02	4.000E+00	250	J023	1 1 2 2 0	
3.236E-04	4.278E-02	ns	D001	0 0 0 0 2	

2108. $C_{10}H_{12}BrCl_2O_3PS$

Bromophos-ethyl
O-(4-Bromo-2,5-dichlorophenyl) *O,O*-diethyl phosphorothioate
Nexagan
Filariol

RN: 4824-78-6 **MP** (°C)**:**
MW: 394.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
8.629E-07	3.400E-04	20	B324	0 0 0 0 0	
8.628E-07	3.400E-04	20	B324	0 0 0 0 0	
7.613E-06	3.000E-03	20	F311	1 2 2 2 1	
5.075E-06	2.000E-03	20	W312	1 0 0 0 0	
1.269E-06	5.001E-04	30	B324	0 0 0 0 0	
1.269E-06	5.000E-04	30	B324	0 0 0 0 0	
5.075E-06	2.000E-03	ns	E050	0 0 0 0 0	
5.075E-06	2.000E-03	rt	M161	0 0 0 0 0	

2109. $C_{10}H_{12}ClNO_2$

Chloro-IPC
Furloe
Taterpex
Chlorpropham
Isopropyl *m*-chlorocarbanilate

RN: 101-21-3 **MP** (°C)**:** 38
MW: 213.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.055E-04	1.080E-01	20	B185	0 0 0 0 0	
3.744E-04	8.000E-02	25	G099	1 0 0 1 0	
3.744E-04	8.000E-02	25	G319	0 0 0 0 0	
4.165E-04	8.900E-02	25	M161	1 0 0 0 1	
3.744E-04	8.000E-02	ns	B185	0 0 0 0 0	
4.119E-04	8.800E-02	ns	B200	0 0 0 0 1	
3.744E-04	8.000E-02	ns	F035	0 0 0 0 0	
4.119E-04	8.800E-02	ns	H042	0 0 0 0 1	
3.744E-04	8.000E-02	ns	M061	0 0 0 0 1	
3.548E-04	7.581E-02	ns	M163	0 0 0 0 0	EFG
5.055E-04	1.080E-01	ns	N013	0 0 0 0 2	

2110. $C_{10}H_{12}ClNO_2$
Baclofen
Lioresal
β-(Aminomethyl)-*p*-chlorohydrocinnamic acid
RN: 1134-47-0 **MP** (°C)**:**
MW: 213.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-02	4.549E+00	25	M374	1 0 2 1 2	

2111. $C_{10}H_{12}ClN_3O_2$
Tranid
3-Chloro-6-cyanonorbornanone-2-oxime-*O,N*-methylcarbamate
RN: 15271-41-7 **MP** (°C)**:** 143.5
MW: 241.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.259E-03	1.996E+00	ns	M061	0 0 0 0 0	

2112. $C_{10}H_{12}ClN_3O_3S$
Quinethazone
7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinazolinesulfonamide
Hydromox
CL 36010
Aquamox
RN: 73-49-4 **MP** (°C)**:** 251
MW: 289.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-04	1.500E-01	25	A081	1 0 1 1 0	EFG

2113. $C_{10}H_{12}ClN_5O_2$
2-Chloro-2′,3′-dideoxyadenosine
2-CIDDA
RN: 114849-58-0 **MP** (°C)**:**
MW: 269.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.745E-03	1.010E+00	25	A336	0 0 0 0 0	

2114. $C_{10}H_{12}Cl_2O$

2,4-Dichloro-6-butyl-phenol
Phenol, 2-butyl-4,6-dichloro-
RN: 91399-13-2 **MP** (°C)**:**
MW: 219.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.259E-02	25	B316	0 0 0 0 0	

2115. $C_{10}H_{12}Cl_3O_2PS$

Trichloronate
Trichloronat
Ethyl *O*-(2,4,5-trichlorophenyl) ethylphosphonothioate
Agritox
Bay 37289
RN: 327-98-0 **MP** (°C)**:**
MW: 333.60 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
1.769E-06	5.901E-04	20	B300	2 1 1 1 2	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
1.499E-04	5.000E-02	20	M161	1 0 0 0 1	*sic*
3.208E-06	1.070E-03	30	B324	0 0 0 0 0	
3.207E-06	1.070E-03	30	B324	0 0 0 0 0	

2116. $C_{10}H_{12}N_2O_2$

Acetone *N*-(phenylcarbamoyl)oxime
Acetone oxime *N*-phenylcarbamate
Proxypham
RN: **MP** (°C)**:** 109.5
MW: 192.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.601E-03	5.000E-01	ns	M061	0 0 0 0 2	approximate

2117. $C_{10}H_{12}N_2O_3$

Barbituric-2-14C acid, 5,5-diallyl
RN: 112599-90-3 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.381E-03	1.745E+00	25	P350	0 0 0 0 0	intrinsic

2118. $C_{10}H_{12}N_2O_3$
Allobarbital
5,5-Diallylbarbituric acid
RN: 52-43-7 **MP** (°C)**:** 171
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.003E-03	1.250E+00	20	J030	1 2 2 2 2	
7.193E-03	1.498E+00	25	A023	1 0 0 1 2	
8.500E-03	1.770E+00	25	G003	1 1 1 1 1	pH 4.7
8.650E-03	1.801E+00	25	V033	2 0 1 1 2	
8.700E-03	1.812E+00	25.00	T303	1 0 0 0 1	
9.250E-03	1.926E+00	30	G014	1 1 1 1 0	EFG
9.200E-03	1.916E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
9.200E-03	1.916E+00	30	K108	1 2 2 0 1	
1.150E-02	2.394E+00	35	A023	1 0 0 1 2	
1.110E-02	2.311E+00	35.00	T303	1 0 0 0 2	
1.215E-02	2.530E+00	37	J030	1 2 2 2 2	
1.200E-02	2.499E+00	37	K121	1 2 1 2 1	0.1N HCl
1.675E-02	3.488E+00	40	A023	1 0 0 1 2	
1.370E-01	2.853E+01	40	N008	1 0 1 1 2	*sic*
1.690E-02	3.519E+00	45.00	T303	1 0 0 0 2	
7.036E-03	1.465E+00	ns	T003	0 0 0 0 2	

2119. $C_{10}H_{12}N_2O_3S$
Bentazon
2,1,3-Benzothiadiazin-4(3H)-one
Thiadiazinol
Basagran 4E
Adagio
BAS 351H
RN: 25057-89-0 **MP** (°C)**:** 138.0
MW: 240.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-03	5.000E-01	20	M161	1 0 0 0 2	
2.080E-03	4.998E-01	ns	B100	0 0 0 0 0	
3.329E-03	8.000E-01	ns	M110	0 0 0 0 0	EFG

2120. $C_{10}H_{12}N_2O_4$
Stavudine
1-(2,3-Dideoxy-β-D-glycero-pent-2-enofuranosyl)thymine
BMY-27857
d4T
Zerit
3′-Deoxy-2′-thymidinene
RN: 3056-17-5 **MP** (°C)**:** 159–160
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-01	7.519E+01	20.5	M439	0 0 0 0 0	
3.791E-01	8.500E+01	24.8	M439	0 0 0 0 0	
4.238E-01	9.502E+01	29.4	M439	0 0 0 0 0	
4.668E-01	1.047E+02	33.2	M439	0 0 0 0 0	
5.563E-01	1.247E+02	38.4	M439	0 0 0 0 0	
3.702E-01	8.300E+01	ns	K444	0 0 0 0 0	
3.418E-01	7.664E+01	ns	S469	0 0 0 0 0	

2121. $C_{10}H_{12}N_2O_4S$
*N*1,*N*4-Diacetylsulfanilamide
*N*4-Acetylsulphacetamide
RN: 5626-90-4 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.389E-03	2.150E+00	37	L091	1 0 0 0 2	pH 5.5

2122. $C_{10}H_{12}N_2O_5$
D-Monofeniltartramide tartranilamide
RN: **MP** (°C)**:** 226
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-02	4.704E+00	21.50	C070	1 2 2 1 2	

2123. $C_{10}H_{12}N_2O_5$

2,4-Dinitro-6-*sec*-butylphenol
Dinoseb
4,6-Dinitro-2-*S*-butylphenol
Phenol, 4,6-dinitro-2-*sec*-butyl-

RN: 88-85-7 **MP** (°C)**:** 38
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.165E-04	5.200E-02	25	B200	1 0 0 0 1	
2.165E-04	5.200E-02	25	G319	0 0 0 0 0	
3.053E-03	7.335E-01	25	M061	1 0 0 0 2	
4.159E-03	9.990E-01	ns	B100	0 0 0 0 0	
2.081E-04	5.000E-02	ns	B185	0 0 0 0 0	
1.413E-03	3.393E-01	ns	M163	0 0 0 0 0	EFG
2.165E-04	5.200E-02	ns	V414	0 0 0 0 0	
4.163E-04	1.000E-01	rt	M161	0 0 0 0 2	

2124. $C_{10}H_{12}N_2O_5S$

7-Aminocephalosporanic acid
7-ACA

RN: 957-68-6 **MP** (°C)**:**
MW: 272.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.901E-04	2.696E-01	1.29	W417	0 0 0 0 0	
1.070E-03	2.914E-01	5.19	W417	0 0 0 0 0	
1.130E-03	3.076E-01	8.29	W417	0 0 0 0 0	
1.255E-03	3.416E-01	12.19	W417	0 0 0 0 0	
1.367E-03	3.723E-01	17.59	W417	0 0 0 0 0	
1.504E-03	4.096E-01	22.99	W417	0 0 0 0 0	
1.627E-03	4.429E-01	27.99	W417	0 0 0 0 0	

2125. $C_{10}H_{12}N_3O_3PS_2$

Azinphos-methyl
Guthion
S-(3,4-Dihydro-4-oxobenzo[d][1,2,3]triazin-3-ylmethyl) *O,O*-dimethyl phosphorodithioate
Methyl gusathion

RN: 86-50-0 **MP** (°C)**:** 74
MW: 317.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.994E-05	9.501E-03	10	B324	0 0 0 0 0	
2.994E-05	9.500E-03	10	B324	0 0 0 0 0	
4.412E-05	1.400E-02	15	A087	1 0 0 1 0	
6.587E-05	2.090E-02	20	B300	2 1 1 1 2	

(*continued*)

2125. $C_{10}H_{12}N_3O_3PS_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.587E-05	2.090E-02	20	B324	0 0 0 0 0	
6.586E-05	2.090E-02	20	B324	0 0 0 0 0	
9.454E-05	3.000E-02	20	M061	1 0 0 0 1	
9.139E-05	2.900E-02	25	A087	1 0 0 1 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.481E-04	4.700E-02	35	A087	1 0 0 1 0	
8.913E-05	2.828E-02	ns	R427	0 0 0 0 0	
1.040E-04	3.300E-02	rt	M161	0 0 0 0 1	

2126. $C_{10}H_{12}N_4$

6,7-Diethylpteridine

RN: **MP** (°C)**:** 52

MW: 188.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.641E-01	1.250E+02	20	A019	2 2 1 1 0	

2127. $C_{10}H_{12}N_4O$

2-Hydroxy-6,7-diethylpteridine
2-Hydroxy-6:7-diethylpteridine
4-Hydroxy-6,7-diethylpteridine
4-Hydroxy-6:7-diethylpteridine

RN: 90870-76-1 **MP** (°C)**:**

MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.494E+00	20	A019	2 2 1 1 2	
5.434E-03	1.110E+00	20	A019	2 2 1 1 2	

2128. $C_{10}H_{12}N_4O_2$

2,4-Dihydroxy-6,7-diethylpteridine
2,4-Dihydroxy-6:7-diethylpteridine

RN: 113222-29-0 **MP** (°C)**:** 218

MW: 220.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.124E-03	9.083E-01	20	A019	2 2 1 1 2	

2129. $C_{10}H_{12}N_4O_2$
1H-Pyrazolo[3,4-d]pyrimidine, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-
2-Tetrahydropuran-4-allopurinyl ether
RN: 52717-52-9 **MP** (°C)**:**
MW: 220.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-02	3.640E+00	ns	H067	0 0 0 0 0	

2130. $C_{10}H_{12}N_4O_2S$
Sulfaethidole
Ethyl thiodiazole
Sulfaethylthiadiazole
Thiodiazolique ethyle
RN: 94-19-9 **MP** (°C)**:** 188
MW: 252.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.522E-04	2.150E-01	20	F073	1 2 2 2 2	
1.288E-02	3.250E+00	37	B046	1 0 2 2 2	pH 5
1.585E-03	4.000E-01	37	D084	1 0 1 0 1	

2131. $C_{10}H_{12}N_4O_3$
1-Butyryloxymethyl allopurinol
Butanoic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-21-5 **MP** (°C)**:** 224–226
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.482E-03	3.500E-01	22	B322	0 0 0 0 0	

2132. $C_{10}H_{12}N_4O_3$
2′,3′-Dideoxyinosine
Videx
Didanosine
CCRIS 805
CCRIS 805Didanosine
RN: 69655-05-6 **MP** (°C)**:** 175
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.614E-02	1.090E+01	4	A337	0 0 0 0 0	
1.156E-01	2.730E+01	25	A337	0 0 0 0 0	
1.270E-01	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic
1.156E-01	2.730E+01	ns	K444	0 0 0 0 0	
1.125E-01	2.657E+01	ns	S469	0 0 0 0 0	

2133. $C_{10}H_{12}N_4O_3$
2-Butyryloxymethyl allopurinol
Butanoic acid, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-22-6 **MP** (°C)**:** 182–183
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.500E+00	22	B322	0 0 0 0 0	

2134. $C_{10}H_{12}N_4O_4$
2′-Deoxy-inosine
2[-Deoxyinosine
Deoxyinosine
RN: 890-38-0 **MP** (°C)**:**
MW: 252.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.301E-02	8.326E+00	25.02	T420	0 0 0 0 0	

2135. $C_{10}H_{12}N_4O_5$
Inosine
Inosin
Hypoxanthine ribonucleoside
RN: 58-63-9 **MP** (°C)**:** 212dec
MW: 268.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.871E-02	1.575E+01	20	D041	1 0 0 0 1	
5.890E-02	1.580E+01	20	F300	1 0 0 0 2	
5.888E-02	1.579E+01	ns	R427	0 0 0 0 0	

2136. $C_{10}H_{12}N_4O_6$
2,4,6-Trinitrodiethylaniline
2-4-6-Trinitrodiethylaniline
RN: 106415-21-8 **MP** (°C)**:**
MW: 284.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.759E-04	5.000E-02	50	D067	1 2 0 0 0	
7.037E-04	2.000E-01	100	D067	1 2 0 0 1	

2137. $C_{10}H_{12}N_5O_6P$
Adenosine 3′:5′-monophosphate
Adenosine, cyclic 3′,5′-(hydrogen phosphate)
4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, adenosine deriv
RN: 60-92-4 **MP** (°C)**:**
MW: 329.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-02	7.769E+00	20	D034	0 0 0 0 0	pH 7.0

2138. $C_{10}H_{12}N_6O_2S$
2-*S*-Cysteinyl-4,6-*bis*-(dimethylamino)-*s*-triazine
RN: **MP** (°C)**:** 173
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.991E-03	2.240E+00	25	C051	1 2 1 1 2	pH 7

2139. $C_{10}H_{12}O$
Estragole
1-Methoxy-4-(2-propen-1-yl)benzene
Chavicyl methyl ether
4-Allylanisole
Tarragon
RN: 140-67-0 **MP** (°C)**:** <25
MW: 148.21 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.778E-01	25	I019	1 0 1 2 2	

2140. $C_{10}H_{12}O$
Anethole
Methoxy-4-propenylbenzene
Propenylanisole
p-Propenylanisole
Anise camphor
Isoestragole
RN: 104-46-1 **MP** (°C)**:** 21.4
MW: 148.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.482E-01	25	D407	1 0 2 2 2	
7.490E-04	1.110E-01	25	I019	1 0 1 2 2	
7.413E-04	1.099E-01	ns	S460	0 0 0 0 0	

2141. $C_{10}H_{12}O$
5,6,7,8-Tetrahydro-2-naphthol
5,6,7,8-Tetrahydro-naphthol-(2)
RN: 1125-78-6 **MP** (°C)**:** 56.5
MW: 148.21 **BP** (°C)**:** 275.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.500E+00	20	F300	1 0 0 0 1	

2142. $C_{10}H_{12}O_2$
Eugenol
1-Allyl-3-methoxy-4-hydroxybenzene
2-Methoxy-4-allylphenol
2-Methoxy-4-(2-propenyl)phenol
4-Allylguaiacol
Allylguaiacol
RN: 97-53-0 **MP** (°C)**:** 15
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-02	2.463E+00	25	I019	1 0 1 2 2	
4.020E-02	6.601E+00	37	E028	1 0 1 1 2	

2143. $C_{10}H_{12}O_2$
Ethyl 2-phenylacetate
Phenylacetic acid ethyl ester
Ethyl benzeneacetate; ethyl phenacetate
NSC 8894
NSC 406259
Ethyl phenylacetate
RN: 101-97-3 **MP** (°C)**:**
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-03	1.478E+00	25	D407	1 0 2 2 2	
8.995E-03	1.477E+00	ns	S460	0 0 0 0 0	

2144. $C_{10}H_{12}O_2$
β-Phenylbutyric acid
3-Phenyl-*n*-butyric acid
RN: 4593-90-2 **MP** (°C)**:** 38
MW: 164.21 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	9.254E+00	30	D033	2 2 1 2 2	
7.013E-02	1.152E+01	40	D033	2 2 1 2 2	

2145. $C_{10}H_{12}O_2$

b-Phenylethanol acetate
Phenylethyl ethanoate
b-Phenylethyl acetate
2-Phenethyl acetate; 2-phenylethyl acetate
Benzylcarbinyl acetate
NSC 71927

RN: 103-45-7 **MP** (°C)**:**
MW: 164.21 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.135E+00	25	D407	1 0 2 2 2	
1.300E-02	2.135E+00	ns	S460	0 0 0 0 0	

2146. $C_{10}H_{12}O_2$

2,4,6-Trimethylbenzoic acid
Mesitylenecarboxylic acid

RN: 480-63-7 **MP** (°C)**:** 154
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-03	7.225E-01	ns	C014	0 2 0 1 1	

2147. $C_{10}H_{12}O_2$

n-Propyl benzoate
Propyl benzoate
Benzoicacidpropyl ester

RN: 2315-68-6 **MP** (°C)**:** –51
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E-03	2.514E-01	20	H301	0 0 0 0 0	

2148. $C_{10}H_{12}O_3$

Anisyl acetate
4-Methoxybenzyl acetate
Benzenemethanol, 4-methoxy-, acetate

RN: 104-21-2 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	1.982E+00	25	D407	1 0 2 2 2	

2149. $C_{10}H_{12}O_3$
Propylparaben
Pr-paraben
Propyl *p*-hydroxybenzoic acid
Propyl 4-hydroxybenzoate
Propyl paraben
RN: 94-13-3 **MP** (°C)**:** 96.5
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.050E-03	3.694E-01	15	B355	0 0 0 0 0	
1.172E-03	2.112E-01	15	M352	1 1 1 1 2	
2.410E-03	4.343E-01	20	B355	0 0 0 0 0	
2.055E-03	3.703E-01	25	A059	1 0 1 1 1	
2.570E-03	4.631E-01	25	B355	0 0 0 0 0	
2.773E-03	4.998E-01	25	D081	1 2 2 1 2	
1.990E-03	3.586E-01	25	D339	0 0 0 0 0	
1.778E-03	3.205E-01	25	F322	2 0 1 1 0	EFG
1.844E-03	3.323E-01	25	M352	1 1 1 1 2	
2.775E-03	5.000E-01	25	O027	1 0 1 0 0	
2.863E-03	5.160E-01	25	P013	0 0 0 0 0	
2.300E-03	4.145E-01	27	B129	2 2 2 2 1	
2.443E-03	4.403E-01	30	A059	1 0 1 1 1	
2.053E-03	3.700E-01	30	M325	1 0 0 0 1	
3.054E-03	5.503E-01	35	A059	1 0 1 1 1	
3.403E-03	6.132E-01	39.3	G302	2 2 2 2 0	EFG
4.053E-03	7.303E-01	40	A059	1 0 1 1 1	
3.925E-03	7.073E-01	40	M352	1 1 1 1 2	
6.492E-03	1.170E+00	50	M352	1 1 1 1 2	
1.515E-03	2.729E-01	ns	B404	0 2 1 1 0	

2150. $C_{10}H_{12}O_4$
Cantharidin
Dimethyl-3,6-epoxyperhydrophthalic anhydride
Cantharides
Hexahydro-3α,7α-dimethyl-4β,7β-epoxyisobenzofuran-1,3-dione
Spanish fly
RN: 56-25-7 **MP** (°C)**:**
MW: 196.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	3.000E-02	20	F300	1 0 0 0 0	
3.058E-01	6.000E+01	100	F300	1 0 0 0 0	
1.514E-04	2.970E-02	ns	R427	0 0 0 0 0	

2151. $C_{10}H_{12}O_5$

Propyl gallate
3,4,5-Trihydroxybenzoic acid propyl ester
Gallic acid propyl ester
Progallin P
n-propyl 3,4,5-trihydroxybenzoate
Nipa 49

RN: 121-79-9 **MP** (°C)**:** 150 C
MW: 212.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-02	2.792E+00	19.99	L430	0 0 0 0 0	
1.644E-02	3.488E+00	24.99	L430	0 0 0 0 0	
1.784E-02	3.786E+00	29.99	L430	0 0 0 0 0	
3.276E-02	6.951E+00	34.99	L430	0 0 0 0 0	
4.850E-02	1.029E+01	39.99	L430	0 0 0 0 0	
7.010E-02	1.488E+01	44.99	L430	0 0 0 0 0	
2.321E-01	4.925E+01	49.99	L430	0 0 0 0 0	
1.158E-01	2.458E+01	49.99	L430	0 0 0 0 0	
6.751E-01	1.432E+02	59.99	L430	0 0 0 0 0	
1.111E+00	2.357E+02	64.99	L430	0 0 0 0 0	
5.648E-03	1.199E+00	–.0	L430	0 0 0 0 0	

2152. $C_{10}H_{12}O_8$

Dilactone
α-Oxo-β-methylol-γ-butyrolactone betrachten

RN: **MP** (°C)**:** 140
MW: 260.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.374E-02	2.439E+01	0	F023	1 1 0 0 1	unit assumed
1.900E-01	4.943E+01	25	F023	1 1 0 0 1	unit assumed
5.972E-01	1.554E+02	50	F023	1 1 0 0 2	unit assumed
1.788E+00	4.652E+02	75	F023	1 1 0 0 2	unit assumed
2.451E+00	6.377E+02	100	F023	1 1 0 0 2	unit assumed

2153. $C_{10}H_{13}ClN_2$
Chlordimeform
N′-(4-Chloro-2-methylphenyl)-*N,N*-dimethylmethanimidamide
Bermat
Fundex
Galecon
Chlorophenamidine
RN: 6164-98-3 **MP** (°C)**:** 32
MW: 196.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.373E-03	2.700E-01	20	B300	2 0 1 1 2	
1.373E-03	2.700E-01	20	B324	0 0 0 0 0	
1.372E-03	2.699E-01	20	B324	0 0 0 0 0	
1.271E-03	2.500E-01	20	M161	1 0 0 0 2	

2154. $C_{10}H_{13}ClN_2O$
Trimeturon
N′-4-Chlorophenyl-*O,N,N*-trimethylisourea
RN: 3050-27-9 **MP** (°C)**:** 147.5
MW: 212.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.289E-03	6.995E-01	ns	M061	0 0 0 0 1	

2155. $C_{10}H_{13}ClN_2O$
Chlortoluron
N′-(3-Chloro-4-methylphenyl)-*N,N*-dimethylurea
Dicuran
Chlortokem
Tolurex
RN: 15545-48-9 **MP** (°C)**:** 147.5
MW: 212.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	7.043E-02	20	B179	0 0 0 0 0	
3.291E-04	7.000E-02	20	F311	1 2 2 2 1	
3.291E-04	7.000E-02	20	M161	1 0 0 0 1	

2156. $C_{10}H_{13}ClN_2O_2$

Metoxuron
N′-(3-Chloro-4-methoxyphenyl)-*N,N*-dimethylurea
Purivel
Sulerex
Dosanex
Dosaflo

RN: 19937-59-8 **MP** (°C)**:** 125
MW: 228.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.906E-01	20	B179	0 0 0 0 0	
2.622E-03	5.996E-01	20	E048	1 2 1 1 2	
2.965E-03	6.780E-01	23	M161	0 0 0 0 2	
3.059E-03	6.995E-01	ns	B100	0 0 0 0 0	

2157. $C_{10}H_{13}ClN_2O_3S$

Chlorpropamide
*N*3-Butyl-*N*1-*p*-chlorobenzenesulfonylurea
Diabinese
Glucamide
Catanil
Diabaril

RN: 94-20-2 **MP** (°C)**:** 128
MW: 276.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.221E-03	8.913E-01	25	F415	0 0 0 0 0	
9.311E-04	2.577E-01	37	A028	1 0 2 1 2	intrinsic
9.250E-04	2.560E-01	37	A046	2 0 1 1 2	
~1.26E-03	~3.50E-01	37	B140	2 2 1 2 0	pH 1.5, form V
1.203E-03	3.330E-01	37	B140	2 2 1 2 2	pH 1.5, form I
1.384E-03	3.830E-01	37	B140	2 2 1 2 2	pH 1.5, form II
8.925E-04	2.470E-01	37	B140	2 2 1 2 2	pH 1.5, form III
1.153E-03	3.190E-01	37	B140	2 2 1 2 2	pH 1.5, form IV
>1.81E-03	>5.00E-01	ns	B404	0 2 1 1 0	
5.192E-04	1.437E-01	rt	I404	0 0 0 0 0	Average

2158. $C_{10}H_{13}Cl_2FN_2O_2S_2$
Tolylfluanid
1,1-Dichloro-*N*-((dimethylamino)sulfonyl)-1-fluoro-*N*-(4-methylphenyl)methanesulfenamide
Dichlofluanid-methyl
Euparen M
Bay 5712α
Bay 49854
RN: 731-27-1 **MP** (°C)**:** 96
MW: 347.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.570E-06	8.926E-04	ns	R427	0 0 0 0 0	
1.152E-02	4.000E+00	rt	M161	0 0 0 0 0	

2159. $C_{10}H_{13}Cl_2O_3PS$
Dichlofenthion
Diethyl *O*-dichlorophenyl phosphorothioate
Hexanema
Diclophenthion
Nemacide
TRI-VC13
RN: 97-17-6 **MP** (°C)**:**
MW: 315.16 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.774E-07	2.450E-04	25	M161	1 0 0 0 2	
7.774E-07	2.450E-04	ns	F071	0 1 2 1 2	
7.774E-04	2.450E-01	ns	M061	0 0 0 0 2	*sic*

2160. $C_{10}H_{13}FN_2O_3$
1-Pivaloyloxymethyl-5-fluorouracil
RN: **MP** (°C)**:**
MW: 228.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	2.500E+00	22	M317	1 1 1 1 1	

2161. $C_{10}H_{13}FN_2O_4$
1-Pivaloyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Pivaloyloxymethyl-5-fluorouracil
RN: 62113-42-2 **MP** (°C)**:** 158-160
MW: 244.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-03	2.300E+00	22	B321	0 0 0 0 0	pH 4.0

2162. $C_{10}H_{13}NO_2$
Phenacetin
p-Ethoxyacetanilide
p-Acetophenetidide
RN: 62-44-2 **MP** (°C)**:** 134.5
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.010E-04	5.395E-02	14	O019	1 0 0 1 2	
2.010E-03	3.603E-01	15	M352	1 1 1 1 2	
3.903E-03	6.995E-01	20	M043	1 0 0 0 0	
5.167E-03	9.261E-01	25	B434	0 0 0 0 0	
5.180E-03	9.284E-01	25	B434	0 0 0 0 0	
4.300E-02	7.706E+00	25	D044	0 0 0 0 0	
4.464E-03	8.000E-01	25	F300	1 0 0 0 0	
2.801E-03	5.020E-01	25	M333	1 1 0 0 2	
2.799E-03	5.016E-01	25	M352	1 1 1 1 2	
6.271E-03	1.124E+00	30	B434	0 0 0 0 0	
6.280E-03	1.126E+00	30	B434	0 0 0 0 0	
8.653E-03	1.551E+00	35	B434	0 0 0 0 0	
8.680E-03	1.556E+00	35	B434	0 0 0 0 0	
1.183E-02	2.120E+00	40	B434	0 0 0 0 0	
1.185E-02	2.124E+00	40	B434	0 0 0 0 0	
5.483E-03	9.828E-01	40	M352	1 1 1 1 2	
7.878E-03	1.412E+00	50	M352	1 1 1 1 2	
6.616E-02	1.186E+01	100	I315	0 0 0 0 0	
7.867E-02	1.410E+01	100	M043	1 0 0 0 2	
4.237E-03	7.594E-01	c	I315	0 0 0 0 0	
6.584E-03	1.180E+00	ns	F059	1 0 2 2 2	0.1N HCl
5.574E-03	9.990E-01	rt	D021	0 0 1 1 1	

2163. $C_{10}H_{13}NO_2$
Propham
Isopropyl carbanilate
Isopropyl-*N*-phenyl carbamate
IPC
RN: 122-42-9 **MP** (°C)**:** 87
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.580E-04	1.000E-01	25	G099	1 0 0 1 0	
1.116E-04	2.000E-02	ns	B185	0 0 0 0 0	
1.786E-04	3.200E-02	ns	B185	0 0 0 0 0	
1.395E-03	2.500E-01	ns	B200	0 0 0 0 2	
5.580E-04	1.000E-01	ns	F035	0 0 0 0 0	
1.395E-03	2.500E-01	ns	H042	0 0 0 0 2	
1.000E-03	1.792E-01	ns	M163	0 0 0 0 0	EFG
1.395E-03	2.500E-01	ns	N013	0 0 0 0 2	

2164. $C_{10}H_{13}NO_2$
Butyl nicotinate
n-Butyl nicotinate
RN: 6938-06-3 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-02	2.450E+00	32	L346	1 0 0 1 2	

2165. $C_{10}H_{13}NO_2$
Propyl-*p*-aminobenzoate
Risocaine
4-Aminobenzoic acid propyl ester
RN: 94-12-2 **MP** (°C)**:** 75.5
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.655E-03	2.966E-01	15	M352	1 1 1 1 2	
2.220E-03	3.979E-01	25	H008	0 0 0 0 0	
2.860E-03	5.125E-01	25	M352	1 1 1 1 2	
3.553E-03	6.368E-01	25	P303	0 0 0 0 0	
4.219E-03	7.561E-01	33	P303	0 0 0 0 0	
4.700E-03	8.423E-01	37	F006	1 1 2 2 2	
4.629E-03	8.297E-01	40	M352	1 1 1 1 2	
5.217E-03	9.351E-01	40	P303	0 0 0 0 0	
7.047E-03	1.263E+00	50	M352	1 1 1 1 2	
1.890E-03	3.387E-01	ns	M066	0 0 0 0 2	
1.890E-03	3.387E-01	rt	B016	0 0 1 1 2	pH 7.4

2166. $C_{10}H_{13}NO_2$
3,4-Xylyl methylcarbamate
3,4-Dimethylphenyl methylcarbamate
3,4-Dimethylphenyl *N*-methylcarbamate
MPMC
Meobal
RN: 2425-10-7 **MP** (°C)**:** 79.5
MW: 179.22 **BP** (°C)**:** 126.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.254E-03	1.300E+00	30	M161	1 0 0 0 1	

2167. $C_{10}H_{13}NO_2$
2,6-Dimethyl-4-acetaminophenol
4-Acetamido-2,6-dimethylphenol
RN: 22900-79-4 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-02	2.200E+00	25	D078	1 2 1 1 2	

2168. $C_{10}H_{13}NO_2$
Methyl *p*-dimethylaminobenzoic acid
Methyl 4-dimethylaminobenzoate
RN: 1202-25-1 **MP** (°C)**:** 371.7
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	6.093E-02	15	M352	1 1 1 1 2	
4.988E-04	8.940E-02	25	M352	1 1 1 1 2	
8.277E-04	1.483E-01	40	M352	1 1 1 1 2	
1.111E-03	1.991E-01	50	M352	1 1 1 1 2	

2169. $C_{10}H_{13}NO_2$
2,5-Dimethyl-4-acetaminophenol
4-Acetamido-2,5-dimethylphenol
RN: 69477-71-0 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-03	1.737E+00	25	D078	1 2 1 1 2	

2170. $C_{10}H_{13}NO_3$
o-Ethoxyphenyl *N*-methylcarbamate
1,2-Ethoxyphenyl *N*-methylcarbamate
RN: 23409-17-8 **MP** (°C)**:** 79.5
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.178E-02	2.300E+00	30	D089	2 2 0 0 0	

2171. $C_{10}H_{13}NO_3$
m-Ethoxyphenyl *N*-methylcarbamate
1,3-Ethoxyphenyl *N*-methylcarbamate
RN: 7225-96-9 **MP** (°C)**:** 57
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.403E-03	1.250E+00	30	D089	2 2 0 0 0	

2172. $C_{10}H_{13}NO_4$
Methyldopa
α-Methyldopa
Sembrina
Presinol
Sedometil
Presolisin
RN: 555-30-6 **MP** (°C)**:** ~300
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.734E-02	1.000E+01	ns	K444	0 0 0 0 0	

2173. $C_{10}H_{13}N_3O_2S_2$
3-Methyl-2-sulfanilamide-2,3-dihydrothiazole
Benzenesulfonamide, 4-amino-*N*-(2,3-dihydro-3-methyl-2-thiazolyl)-
RN: 51203-20-4 **MP** (°C)**:**
MW: 271.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.690E-04	1.544E-01	37	K095	2 0 0 0 2	intrinsic

2174. $C_{10}H_{13}N_3O_5S$
Nifurtimox
4-((5-Nitrofurfurylidene)amino)-3-methylthiomorpholine-1,1-dioxide
RN: 23256-30-6 **MP** (°C)**:**
MW: 287.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.149E-01	3.300E+01	ns	K444	0 0 0 0 0	

2175. $C_{10}H_{13}N_4O_3$
Spasmolysin
β-Hydroxypropyltheophylline
RN: 603-00-9 **MP** (°C)**:**
MW: 237.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E+00	2.857E+02	ns	J025	0 0 0 0 1	

2176. $C_{10}H_{13}N_5$
4-Amino-6,7-diethylpteridine
RN: **MP** (°C)**:**
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.171E-03	2.380E-01	20	A019	2 2 1 1 2	

2177. $C_{10}H_{13}N_5$
2-Amino-6,7-diethylpteridine
RN: **MP** (°C)**:**
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.110E-04	1.852E-01	20	A019	2 2 1 1 2	

2178. $C_{10}H_{13}N_5O$
2-Amino-4-hydroxy-6,7-diethylpteridine
2-Amino-4-hydroxy-6:7-diethylpteridine
RN: **MP** (°C)**:** >350
MW: 219.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-05	1.163E-02	20	A019	2 2 1 1 2	

2179. $C_{10}H_{13}N_5O$
4-Amino-2-hydroxy-6,7-diethylpteridine
4-Amino-2-hydroxy-6:7-diethylpteridine
RN: **MP** (°C)**:**
MW: 219.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.850E-04	6.250E-02	20	A019	2 2 1 1 2	

2180. $C_{10}H_{13}N_5O_2$
2′,3′-Dideoxyadenosine
DDA
RN: 4097-22-7 **MP** (°C)**:** 181–184
MW: 235.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.228E-01	2.890E+01	4	A337	0 0 0 0 0	
1.836E-01	4.320E+01	25	A337	0 0 0 0 0	

2181. $C_{10}H_{13}N_5O_3$
Deoxyadenosine
2′-Deoxyadenosine
dA
RN: 958-09-8 **MP** (°C)**:**
MW: 251.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E-02	3.573E+00	14.88	T420	0 0 0 0 0	
1.827E-02	4.590E+00	20.26	T420	0 0 0 0 0	
2.690E-02	6.759E+00	25	H061	0 0 0 0 0	
2.558E-02	6.427E+00	25.23	T420	0 0 0 0 0	
3.683E-02	9.253E+00	29.97	T420	0 0 0 0 0	
4.780E-02	1.201E+01	35.09	T420	0 0 0 0 0	

2182. $C_{10}H_{13}N_5O_4$
Zidovudine
3-Azido-3-deoxythymidine
AZT
Azidodeoxythymidine
Azidothymidine
Retrovir
RN: 30516-87-1 **MP** (°C)**:** 106–112
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.13E+00	>3.02E+02	25	B443	0 0 0 0 0	
7.521E-02	2.010E+01	ns	K444	0 0 0 0 0	
7.373E-02	1.970E+01	ns	S469	0 0 0 0 0	

2183. $C_{10}H_{13}N_5O_4$
Adenosine
Adenosin
9-B-D-Ribofuranosyl-9H-purin-6-amine adenine riboside
Adenocard
9-β-D-Ribofuranosyladenine
RN: 58-61-7 **MP** (°C)**:** 234
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	5.131E+00	25	H061	0 0 0 0 0	
2.000E-02	5.345E+00	ns	R030	0 0 0 0 0	
1.905E-02	5.092E+00	ns	R427	0 0 0 0 0	
8.232E-05	2.200E-02	rt	N015	0 0 2 2 1	*sic*

2184. $C_{10}H_{13}N_5O_4$
Guanine deoxyriboside
RN: 961-07-9 **MP** (°C)**:**
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E-03	1.785E+00	14.88	T420	0 0 0 0 0	
8.790E-03	2.349E+00	20.26	T420	0 0 0 0 0	
1.118E-02	2.988E+00	25.02	T420	0 0 0 0 0	
1.589E-02	4.247E+00	29.97	T420	0 0 0 0 0	
2.072E-02	5.537E+00	35.09	T420	0 0 0 0 0	

2185. $C_{10}H_{13}N_5O_5$
Guanosine
Guanosin
2-Amino-9-β-D-ribofuranosyl-9H-purine-6-(1H)-one
Guanine riboside
rG
RN: 118-00-3 **MP** (°C)**:** 250
MW: 283.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.471E-03	7.000E-01	18	F300	1 0 0 0 1	
4.300E-03	1.218E+00	25	C416	2 1 1 1 1	
1.820E-03	5.155E-01	25	H061	0 0 0 0 0	
1.073E-01	3.040E+01	100	F300	1 0 0 0 1	

2186. $C_{10}H_{14}$
Isobutylbenzene
2-Methyl-1-phenylpropane
(2-Methylpropyl)-benzene
RN: 538-93-2 **MP** (°C)**:** –51
MW: 134.22 **BP** (°C)**:** 170.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.525E-05	1.010E-02	25	P051	2 1 1 2 2	
7.525E-05	1.010E-02	25.00	P007	2 1 2 2 2	
7.525E-05	1.010E-02	ns	H123	0 0 0 0 0	

2187. $C_{10}H_{14}$
Durene
1,2,4,5-Tetramethylbenzene
Durol
RN: 95-93-2 **MP** (°C)**:** 80.0
MW: 134.22 **BP** (°C)**:** 192.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.593E-05	3.480E-03	25	K119	1 0 0 0 2	
2.593E-05	3.480E-03	25	P051	2 1 1 2 2	
2.593E-05	3.480E-03	25.00	P007	2 1 2 2 2	
1.445E-04	1.940E-02	ns	D001	0 0 0 0 2	
7.152E-05	9.600E-03	ns	H123	0 0 0 0 0	

2188. $C_{10}H_{14}$
Butylbenzene
1-Phenylbutane
n-Butylbenzene
RN: 68411-44-9 **MP** (°C)**:** –88
MW: 134.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.745E+00	ns	H307	0 0 0 0 0	

2189. $C_{10}H_{14}$
n-Butylbenzene
1-Phenylbutane
Butylbenzene
RN: 104-51-8 **MP** (°C)**:** –88.5
MW: 134.22 **BP** (°C)**:** 183.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.940E-05	1.334E-02	7	O312	2 2 0 2 2	
9.670E-05	1.298E-02	10	O312	2 2 0 2 2	
9.790E-05	1.314E-02	12.5	O312	2 2 0 2 2	
9.660E-05	1.297E-02	15	O312	2 2 0 2 2	
9.790E-05	1.314E-02	17.5	O312	2 2 0 2 2	
9.909E-05	1.330E-02	20	B356	0 0 0 0 0	
1.018E-04	1.366E-02	20	O312	2 2 0 2 2	
9.387E-06	1.260E-03	25	A002	1 2 1 1 2	*sic*
3.700E-04	4.966E-02	25	K001	1 0 2 1 2	
1.320E-04	1.772E-02	25	M124	2 1 2 2 2	
1.030E-04	1.382E-02	25	M342	1 0 1 1 2	
1.025E-04	1.376E-02	25	O312	2 2 0 2 2	
8.791E-05	1.180E-02	25	S005	2 2 2 2 2	
3.725E-04	5.000E-02	25	S012	2 0 2 2 0	
8.791E-05	1.180E-02	25	S191	1 2 2 2 2	
8.791E-05	1.180E-02	25	S358	2 1 2 2 2	
1.030E-04	1.382E-02	25	W300	2 2 2 2 2	
1.244E-04	1.670E-02	29.99	C350	0 0 0 0 0	
1.086E-04	1.458E-02	30	O312	2 2 0 2 2	
1.147E-04	1.540E-02	35	O312	2 2 0 2 2	
1.328E-04	1.782E-02	39.99	C350	0 0 0 0 0	
1.234E-04	1.656E-02	40	O312	2 2 0 2 2	
1.411E-04	1.894E-02	45	O312	2 2 0 2 2	
1.517E-04	2.036E-02	49.99	C350	0 0 0 0 0	
2.006E-04	2.692E-02	59.99	C350	0 0 0 0 0	
2.389E-04	3.206E-02	69.99	C350	0 0 0 0 0	
3.555E-04	4.772E-02	79.99	C350	0 0 0 0 0	
4.555E-04	6.114E-02	89.99	C350	0 0 0 0 0	
6.222E-04	8.351E-02	99.99	C350	0 0 0 0 0	
9.387E-05	1.260E-02	ns	H123	0 0 0 0 0	

2190. $C_{10}H_{14}$
p-Cymene
1-Methyl-4-isopropylbenzene
4-Cymene
Dolcymine
RN: 99-87-6 **MP** (°C)**:** –68
MW: 134.22 **BP** (°C)**:** 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-03	3.998E-01	25	B019	1 0 1 2 0	*sic*
1.740E-04	2.335E-02	25	B173	2 0 2 2 2	*sic*

2191. $C_{10}H_{14}$
sec-Butylbenzene
1-Methylpropylbenzene
RN: 135-98-8 **MP** (°C)**:** –82.7
MW: 134.22 **BP** (°C)**:** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.302E-03	3.090E-01	25	A002	1 2 1 1 2	*sic*
7.525E-05	1.010E-02	25	K119	1 0 0 0 2	
1.311E-04	1.760E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
1.311E-04	1.760E-02	25	S358	2 1 2 2 2	

2192. $C_{10}H_{14}$
tert-Butylbenzene
1,1-Dimethylethylbenzene
t-Butylbenzene
RN: 98-06-6 **MP** (°C)**:** –58
MW: 134.22 **BP** (°C)**:** 168.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-04	3.400E-02	25	A002	1 2 1 1 1	
2.198E-04	2.950E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
2.198E-04	2.950E-02	25	S358	2 1 2 2 2	

2193. $C_{10}H_{14}$
1,2-Diethylbenzene
o-Diethylbenzene
RN: 135-01-3 **MP** (°C)**:** –31
MW: 134.22 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	7.114E-02	10	B149	2 1 1 2 1	
5.300E-04	7.114E-02	20	B149	2 1 1 2 1	

2194. $C_{10}H_{14}$
1,4-Diethylbenzene
p-Diethylbenzene
RN: 105-05-5 **MP** (°C)**:** –43
MW: 134.22 **BP** (°C)**:** 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	2.483E-02	10	B149	2 1 1 2 2	
1.850E-04	2.483E-02	20	B149	2 1 1 2 2	

2195. $C_{10}H_{14}Cl_2NO_2PS$
DMPA
Isopropylphosphoramidothioate
O-(2,4-Dichlorophenyl)-*O*-methyl
Phosphoramidothioic acid, isopropyl-*o*-(2,4-dichlorophenyl)-*o*-methyl ester
RN: 299-85-4 **MP** (°C)**:** 51.4
MW: 314.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.595E-05	5.010E-03	25	B185	0 0 0 0 0	
1.591E-05	5.000E-03	25	B200	1 0 0 0 0	
1.591E-05	5.000E-03	ns	M061	0 0 0 0 0	

2196. $C_{10}H_{14}Cl_6N_4O_2$
Triforine
N,N′-[1,4-Piperazinediylbis(2,2,2-trichloroethylidene)] bisformamide
Funginex
Denarin
Biformylchlorazin
Saprol
RN: 26644-46-2 **MP** (°C)**:** 155
MW: 434.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.38E-05	~6.00E-03	rt	D303	0 0 0 0 0	
6.437E-05	2.800E-02	rt	M161	0 0 0 0 0	

2197. $C_{10}H_{14}NO_5PS$
Parathion
O,O-Diethyl *O*-*p*-nitrophenyl phosphorothioate
Foliclal
Rhodiatox
Alkron
Fosferno
RN: 56-38-2 **MP** (°C)**:** 6
MW: 291.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
4.257E-05	1.240E-02	20	B169	2 1 1 1 1	
8.318E-05	2.423E-02	20	B179	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
2.245E-05	6.540E-03	24	F179	2 2 2 2 2	
8.240E-05	2.400E-02	25	M161	1 0 0 0 1	

(*continued*)

2197. $C_{10}H_{14}NO_5PS$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
4.086E-05	1.190E-02	ns	F071	0 1 2 1 2	
8.240E-05	2.400E-02	ns	M061	0 0 0 0 1	
6.867E-05	2.000E-02	ns	M110	0 0 0 0 0	EFG
8.240E-05	2.400E-02	ns	M344	0 0 0 0 1	

2198. $C_{10}H_{14}NO_6P$

Paraoxon
Diethyl *p*-nitrophenyl phosphate
Fosfacol
Eticol
Ethyl paraoxon
Miotisal

RN: 311-45-5 **MP** (°C)**:**
MW: 275.20 **BP** (°C)**:** 169–170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-02	3.627E+00	20	B169	2 0 1 1 2	
3.634E-03	1.000E+00	20	F300	1 0 0 0 0	

2199. $C_{10}H_{14}N_2O$

N-(Dimethylaminomethyl)benzamide
Benzamide, *N*-[(dimethylamino)methyl]-

RN: 59917-58-7 **MP** (°C)**:**
MW: 178.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	4.634E+02	22	J037	0 0 0 0 0	

2200. $C_{10}H_{14}N_2O$

N-(Ethylaminomethyl)benzamide
Benzamide, *N*-[(ethylamino)methyl]-

RN: 73239-20-0 **MP** (°C)**:**
MW: 178.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-02	1.301E+01	22	J037	0 0 0 0 0	

2201. $C_{10}H_{14}N_2O_2$
m-N,N-Dimethylaminophenyl *N*-methylcarbamate
1,3-*N,N*-Dimethylaminophenyl *N*-methylcarbamate
RN: 2631-39-2 **MP** (°C)**:** 86
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.604E-03	7.000E-01	30	D089	2 2 0 0 0	

2202. $C_{10}H_{14}N_2O_3$
5-Methyl-5-(3-methylbut-2-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(3-methyl-2-butenyl)
5-Methyl-5-(3-methylbut-2-enyl)barbiturate
RN: 66843-01-4 **MP** (°C)**:**
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.503E-03	5.262E-01	25	P350	0 0 0 0 0	intrinsic

2203. $C_{10}H_{14}N_2O_3$
2,4-Diazaspiro[5.6]dodecane-1,3,5-trione
Cycloheptane-spirobarbiturate
RN: 143288-61-3 **MP** (°C)**:**
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.790E-04	1.427E-01	25	P350	0 0 0 0 0	intrinsic

2204. $C_{10}H_{14}N_2O_3$
5-Isopropyl-5-allylbarbituric acid
Aprobarbital
5-(1-Methylethyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-isopropylbarbituric acid
Aprobarbitone
RN: 77-02-1 **MP** (°C)**:** 141
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.617E-02	3.400E+00	20	J030	1 2 2 2 2	
1.960E-02	4.121E+00	25	P350	0 0 0 0 0	intrinsic
1.940E-02	4.079E+00	25	V033	2 0 1 1 2	
1.940E-02	4.079E+00	25.00	T303	1 0 0 0 2	
2.600E-02	5.466E+00	35.00	T303	1 0 0 0 2	
2.664E-02	5.600E+00	37	J030	1 2 2 2 2	
3.340E-02	7.022E+00	45.00	T303	1 0 0 0 2	
1.912E-02	4.020E+00	ns	T003	0 0 0 0 2	

2205. $C_{10}H_{14}N_2O_5$
Thymidine
(1-[2-Deoxy-β-D-ribofuranosyl]-5-methyluracil)
Thyminedeoxyriboside
2′-deoxy-5-methyl
Thymine-2-desoxyriboside
Uridine
RN: 50-89-5 **MP** (°C)**:** 187–189
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	6.589E+00	19.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.96	T418	0 0 0 0 0	
2.780E-02	6.734E+00	24.99	T418	0 0 0 0 0	
3.040E-02	7.364E+00	24.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.99	T418	0 0 0 0 0	
2.870E-02	6.952E+00	24.99	T418	0 0 0 0 0	
2.200E-01	5.329E+01	24.99	T418	0 0 0 0 0	
2.710E-02	6.565E+00	25.49	T418	0 0 0 0 0	

2206. $C_{10}H_{14}N_2S$
Methiuron
N,N-Dimethyl-*N′*-3-methylphenylthiourea
RN: 21540-35-2 **MP** (°C)**:** 145
MW: 194.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-03	4.000E-01	ns	M061	0 0 0 0 2	

2207. $C_{10}H_{14}N_4O_2$
7-Propyl theophylline
3,7-Dimethyl-7-propyl-xanthine
RN: 27760-74-3 **MP** (°C)**:**
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E+00	2.320E+02	30	B042	1 2 1 1 2	
1.040E+00	2.311E+02	30	G021	1 0 0 0 2	

2208. $C_{10}H_{14}N_4O_2$
1-Propyl theobromine
3,7-Dimethyl-1-propyl-xanthine
RN: 204443-29-8 **MP** (°C)**:** 99
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.190E-02	1.376E+01	30	B042	1 2 1 1 2	

2209. $C_{10}H_{14}N_4O_3$
Ethoxycaffeine
1,3,7-Trimethyl-2,6-dioxo-8-ethoxypurine
RN: 577-66-2 **MP** (°C)**:** 143
MW: 238.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-02	2.991E+00	19	A072	1 2 1 0 1	

2210. $C_{10}H_{14}N_4O_4$
Dyphylline
7-(2,3-Dihydroxypropyl)theophylline
Lufyllin-EPG
Neothylline
Airet
RN: 479-18-5 **MP** (°C)**:** 158
MW: 254.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-01	1.700E+02	37	F076	2 0 2 2 1	

2211. $C_{10}H_{14}N_5O_7P$
2′-Adenylic acid
2′-Adenylsaeure
RN: 130-49-4 **MP** (°C)**:**
MW: 347.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2212. $C_{10}H_{14}N_5O_7P$
3′-Adenylic acid
3′-Adenylsaeure
RN: 84-21-9 **MP** (°C)**:** 197
MW: 347.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2213. $C_{10}H_{14}O$

L-Carvone
r-(–)-*p*-Mentha-6,8-dien-2-one
1-Methyl-4-isopropenyl-6-cyclohexen-2-one
p-Mentha-6,8-dien-2-one
RN: 6485-40-1 **MP** (°C)**:** <25
MW: 150.22 **BP** (°C)**:** 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.654E-03	1.300E+00	18	F300	1 0 0 0 1	
8.654E-03	1.300E+00	25	A049	1 0 0 0 1	
1.020E-02	1.532E+00	25	A401	1 0 2 2 0	
1.100E-02	1.652E+00	25	D407	1 0 2 2 2	
1.100E-02	1.652E+00	37	E028	1 0 1 1 2	

2214. $C_{10}H_{14}O$

l-Perillaldehyde
4-Isopropenyl-1-cyclohexene-1-carboxaldehyde
para-Mentha-1,8-dien-7-al
L-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde
L(–)-Perillaldehyde
(*S*)-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde
RN: 18031-40-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	6.309E-01	25	A401	1 0 2 2 0	

2215. $C_{10}H_{14}O$

p-*n*-Butylphenol
4-*n*-Butylphenol
RN: 1638-22-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.038E-03	4.563E-01	20	R087	0 0 0 0 0	0.15M NaCl
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2216. $C_{10}H_{14}O$

o-*n*-Butylphenol
2-*n*-Butylphenol
RN: 28805-86-9 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2217. $C_{10}H_{14}O$
p-tert-Butylphenol
4-*t*-Butylphenol
RN: 98-54-4 **MP** (°C)**:** 99.5
MW: 150.22 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.327E-03	6.500E-01	22.5	G301	0 0 0 0 0	
3.327E-03	4.998E-01	25	L021	1 0 0 0 0	
3.861E-03	5.800E-01	25	M127	1 0 0 0 1	
4.427E-03	6.650E-01	25	P004	0 0 0 0 0	
5.076E-03	7.625E-01	30	P004	0 0 0 0 0	
5.785E-03	8.690E-01	35	P004	0 0 0 0 0	
6.534E-03	9.815E-01	40	P004	0 0 0 0 0	
4.266E-03	6.408E-01	ns	R427	0 0 0 0 0	

2218. $C_{10}H_{14}O$
Thymol
6-Isopropyl-*m*-cresol
3-Hydroxy-*p*-cymene
5-Methyl-2-isopropyl-1-phenol
2-Isopropyl-5-methyl phenol
5-Methyl-2-(1-methylethyl)phenol
RN: 89-83-8 **MP** (°C)**:** 48–51
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.991E-03	9.000E-01	20	F300	1 0 0 0 0	
6.000E-03	9.013E-01	25	D407	1 0 2 2 2	
5.700E-03	8.563E-01	25	F044	1 0 0 0 1	
6.046E-03	9.083E-01	25	L021	1 0 0 0 0	
6.650E-03	9.990E-01	25	R041	0 0 0 0 0	
5.990E-02	8.998E+00	37	E028	1 0 1 1 2	*sic*
8.654E-03	1.300E+00	37	F300	1 0 0 0 1	
6.166E-03	9.263E-01	ns	R427	0 0 0 0 0	

2219. $C_{10}H_{14}O$
Carvacrol
2-Methyl-5-isopropylphenol
RN: 499-75-2 **MP** (°C)**:** 3
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-03	9.990E-01	25	L021	1 0 0 0 0	
8.321E-03	1.250E+00	25	M127	1 0 0 0 2	

2220. $C_{10}H_{14}O$
4-*sec*-Butylphenol
p-*sec*-Butylphenol
RN: 99-71-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-03	9.600E-01	25	M127	1 0 0 0 1	

2221. $C_{10}H_{14}O_2$
3-Butoxyphenol
m-Butoxy phenol
Phenol, 3-butoxy-
RN: 18979-72-1 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.240E-03	1.370E+00	30	B315	0 0 0 0 0	

2222. $C_{10}H_{14}O_2$
p-Diethoxybenzene
4-Diethoxybenzene
RN: 122-95-2 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.560E-04	7.580E-02	25	C316	0 0 0 0 0	0.1M NaCl

2223. $C_{10}H_{14}O_2$
o-Butoxyphenol
2-Butoxyphenol
RN: 39075-90-6 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-03	6.516E-01	24.99	B353	0 0 0 0 0	

2224. $C_{10}H_{14}O_8$

1,1,2,2-Ethanetetrol, tetraacetate
Glyoxal-tetraacetat
Glyoxal tetraacetate
RN: 59602-16-3 **MP** (°C)**:**
MW: 262.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-05	8.000E-03	25	F300	1 0 0 0 1	

2225. $C_{10}H_{15}N$

Diethylaniline
2,6-Diethylaniline
RN: 579-66-8 **MP** (°C)**:** –38
MW: 149.24 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.489E-03	6.700E-01	26.70	L095	2 2 1 1 2	
4.467E-03	6.666E-01	ns	S460	0 0 0 0 0	

2226. $C_{10}H_{15}NO$

Ethyl phenyl ethanolamine
2-(*N*-Ethylanilino)ethanol
N-Phenyl-*N*-ethylethanolamine
RN: 92-50-2 **MP** (°C)**:**
MW: 165.24 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-02	4.975E+00	20	M062	1 0 0 0 1	

2227. $C_{10}H_{15}NO$

Ephedrine
L-Erythro-2-(methylamino)-1-phenylpropan-1-ol
(1*R*,2*S*)-(–)-Ephedrine
L-α-(1-Methylaminoethyl)benzyl alcohol
RN: 299-42-3 **MP** (°C)**:** 38–39
MW: 165.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.882E-01	4.762E+01	25	D004	0 0 0 0 0	
3.442E-01	5.688E+01	25	L338	1 0 1 1 2	
3.850E-01	6.362E+01	30	L069	1 0 1 1 0	EFG
1.160E+00	1.917E+02	ns	F007	0 0 0 0 2	

2228. $C_{10}H_{15}NO$
(+)-Pseudoephedrine
(+)-Pseudoephedrin
RN: 90-82-4 **MP** (°C)**:** 118
MW: 165.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.03E-03	<5.00E-01	rt	B435	0 0 0 0 0	

2229. $C_{10}H_{15}NO_2$
N-Phenyldiethanolamine
Phenyl diethanolamine
N,N-di(Hydroxyethyl)aniline
2,2′-(Phenylimino)diethanol
PDEA
RN: 120-07-0 **MP** (°C)**:** 57
MW: 181.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-01	3.232E+01	20	M062	1 0 0 0 2	

2230. $C_{10}H_{15}N_5O_5$
Arabinosyladenine
9-β-D-Arabino furanosyl adenine
Vidarabine
β-D-Arabinosyladenine
Spongoadenosine
RN: 24356-66-9 **MP** (°C)**:** 208
MW: 285.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	5.135E-01	ns	R030	0 0 0 0 0	

2231. $C_{10}H_{15}OPS_2$
Fonofos
Ethyl *S*-phenyl ethylphosphonothiolthionate
Diphonate
Dyfonate®
Stauffer N-2790
RN: 944-22-9 **MP** (°C)**:**
MW: 246.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-05	1.570E-02	20	B169	2 1 1 1 2	
6.089E-05	1.500E-02	ns	M110	0 0 0 0 0	EFG

(*continued*)

2231. $C_{10}H_{15}OPS_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.272E-05	1.299E-02	ns	S460	0 0 0 0 0	
6.374E-05	1.570E-02	ns	V414	0 0 0 0 0	

2232. $C_{10}H_{15}O_3PS_2$

Fenthion
4-Methylmercapto-3-methylphenyl dimethyl thiophosphate
Mercaptofos
Thiophos
Baycid
Entex

RN: 55-38-9 **MP** (°C)**:** 7.5
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-05	6.400E-03	10	B324	0 0 0 0 0	
2.300E-05	6.402E-03	10	B324	0 0 0 0 0	
2.698E-05	7.509E-03	20	B300	2 1 1 1 2	
3.244E-05	9.029E-03	20	B324	0 0 0 0 0	
3.341E-05	9.300E-03	20	B324	0 0 0 0 0	
1.940E-04	5.400E-02	20	M061	1 0 0 0 1	
4.074E-05	1.134E-02	30	B324	0 0 0 0 0	
4.060E-05	1.130E-02	30	B324	0 0 0 0 0	
1.976E-04	5.500E-02	rt	M161	0 0 0 0 0	

2233. $C_{10}H_{16}$

Myrcene
7-Methyl-3-methylene-1,6-octadiene
7-Methyl-3-methylene-1,6-octadiene
7-Methyl-3-methyleneocta-1,6-diene
7-Methyl-3-methylene-octadiene
β-Myrcene

RN: 123-35-3 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	4.087E-03	25	A401	1 0 2 2 0	
7.560E-05	1.030E-02	25	L450	0 0 0 0 0	

2234. $C_{10}H_{16}$
β-Pinene
(10)-Pinene
Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-
Nopinene
Pseudopinene
RN: 127-91-3 **MP** (°C)**:** –61
MW: 136.24 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	1.272E-02	24.99	T424	0 0 0 0 0	
8.808E-05	1.200E-02	25	L450	0 0 0 0 0	

2235. $C_{10}H_{16}$
D-Limonene
D-1,8-*p*-Menthadiene
(*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene
(*R*)-(+)-Limonene
Hemo-sol
RN: 5989-27-5 **MP** (°C)**:** 95
MW: 136.24 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.080E-01	9.646E+01	0	M124	2 1 2 2 1	
7.670E-01	1.045E+02	5	M124	2 1 2 2 2	
6.973E-05	9.500E-03	25	L450	0 0 0 0 0	
1.011E-04	1.377E-02	25	M124	2 1 2 2 1	

2236. $C_{10}H_{16}$
Limonene
p-Mentha-1,8-diene
Cyclil decene
Acintene DP dipentene
RN: 138-86-3 **MP** (°C)**:** 73.97
MW: 136.24 **BP** (°C)**:** 175.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-05	4.332E-03	6	P430	0 0 0 0 0	
4.100E-05	5.586E-03	23.5	P430	0 0 0 0 0	
9.055E-05	1.234E-02	24.99	T424	0 0 0 0 0	
6.390E-05	8.706E-03	25	I019	1 0 1 2 2	
2.202E-04	3.000E-02	25	M350	1 0 1 1 1	

2237. $C_{10}H_{16}$
γ-Terpinene
1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene
1,4-*p*-Menthadiene
1-Isopropyl-4-methyl-1,4-cyclohexadiene
Moslene
Terpinene
RN: 99-85-4 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-05	6.090E-03	6	P430	0 0 0 0 0	
6.370E-05	8.678E-03	23.5	P430	0 0 0 0 0	

2238. $C_{10}H_{16}$
Terpinolene
1-Methyl-4-(1-methylethylidene)cyclohexene
1,4(8)-*p*-Menthadiene
1-Methyl-4-(1-methylethylidene)cyclohexene
Terpinolene 30/35
Terpinolene 90
RN: 586-62-9 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.670E-05	7.725E-03	6	P430	0 0 0 0 0	
6.960E-05	9.482E-03	23.5	P430	0 0 0 0 0	
5.000E-05	6.812E-03	25	A401	1 0 2 2 0	

2239. $C_{10}H_{16}$
α-Pinene
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene
Acitene A
Cyclic dexadiene
pin-2(3)-ene
2-Pinene
RN: 80-56-8 **MP** (°C)**:** –64
MW: 136.24 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-05	2.275E-03	6	P430	0 0 0 0 0	
1.830E-05	2.493E-03	23.5	P430	0 0 0 0 0	
3.867E-05	5.268E-03	24.99	T424	0 0 0 0 0	
3.523E-05	4.800E-03	25	L450	0 0 0 0 0	

2240. $C_{10}H_{16}Cl_3NOS$
Triallate
S-(2,3,3-Trichloroallyl)diisopropylthiocarbamate
RN: 2303-17-5 **MP** (°C)**:** 29
MW: 304.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-05	4.000E-03	25	B200	1 0 0 1 0	
1.313E-05	4.000E-03	25	M161	1 0 0 0 0	
1.313E-05	4.000E-03	ns	F019	0 0 0 0 0	

2241. $C_{10}H_{16}NO_2S_2$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dithiolane
2-Cyclopentyl-4-methoxycarbamyl-1,3-dithiolane
RN: **MP** (°C)**:**
MW: 246.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.391E-02	rt	B174	0 0 1 0 0	

2242. $C_{10}H_{16}NO_3S$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-oxathiolane
RN: **MP** (°C)**:**
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-03	3.455E-01	rt	B174	0 0 1 0 1	

2243. $C_{10}H_{16}NO_4$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dioxolane
RN: **MP** (°C)**:**
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.785E+00	rt	B174	0 0 1 0 1	

2244. $C_{10}H_{16}N_2O_3$
5-Ethyl-5-(2-methylpropyl)barbituric acid
RN: 125-40-6 **MP** (°C)**:** 174.5
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.997E-03	8.483E-01	25	B065	1 2 1 1 1	

2245. $C_{10}H_{16}N_2O_3$
5,5-Dipropylbarbituric acid
5,5-Dipropylbarbitursaeure
Proponal
5,5-Dipropylbarbiturate
RN: 2217-08-5 **MP** (°C)**:** 146
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-03	6.000E-01	20	F300	1 0 0 0 0	
2.968E-03	6.300E-01	20	J030	1 2 2 2 1	
5.088E-03	1.080E+00	37	J030	1 2 2 2 2	
6.926E-02	1.470E+01	100	F300	1 0 0 0 2	

2246. $C_{10}H_{16}N_2O_3$
5,5-Diisopropylbarbituric acid
Barbituric acid, 5,5-diisopropyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-bis(1-methylethyl)
5,5-Di-i-propylbarbiturate
RN: 99167-69-8 **MP** (°C)**:**
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E-03	3.640E-01	25	P350	0 0 0 0 0	intrinsic

2247. $C_{10}H_{16}N_2O_3$
Butabarbital
Butethal
5-Ethyl-5-*n*-butylbarbituric acid
5-Butyl-5-ethylbarbituric acid
RN: 77-28-1 **MP** (°C)**:** 127
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.602E-02	3.400E+00	0	D089	0 0 0 0 2	form I
1.484E-02	3.150E+00	20	J030	1 2 2 2 2	
1.044E-02	2.215E+00	20	K078	1 0 2 1 2	
4.052E-03	8.600E-01	25	B011	2 0 0 1 0	
4.218E-03	8.954E-01	25	B065	1 1 1 1 1	
1.936E-02	4.110E+00	25	B065	1 1 1 1 1	
8.000E-03	1.698E+00	25	G003	1 1 1 1 1	pH 4.7
2.300E-02	4.882E+00	25	M310	2 2 2 2 2	
2.130E-02	4.521E+00	25	V033	2 0 1 1 2	
4.070E-03	8.639E-01	25	V033	2 0 1 1 2	
2.130E-02	4.521E+00	25.00	T303	1 0 0 0 2	
7.400E-03	1.571E+00	25.00	T303	1 0 0 0 1	

(*continued*)

2247. $C_{10}H_{16}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-02	4.139E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
9.900E-03	2.101E+00	35.00	T303	1 0 0 0 1	
2.430E-02	5.158E+00	35.00	T303	1 0 0 0 2	
2.299E-02	4.880E+00	37	J030	1 2 2 2 2	
3.090E-02	6.559E+00	45.00	T303	1 0 0 0 2	
1.370E-02	2.908E+00	45.00	T303	1 0 0 0 2	
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form II
1.602E-02	3.400E+00	amb	D092	0 2 2 1 2	0.1N HCl, form III, mp 124 C
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form I
9.362E-03	1.987E+00	ns	T003	0 0 0 0 2	
8.952E-03	1.900E+00	ns	T003	0 0 0 0 2	

2248. $C_{10}H_{16}N_2O_3S$

Biotin d
D-Biotin
Biotin

RN: 58-85-5 **MP** (°C)**:** 232
MW: 244.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.003E-04	2.200E-01	25	D041	1 0 0 0 1	
1.433E-03	3.500E-01	25	D315	0 0 0 0 0	
8.186E-04	2.000E-01	25	M054	1 0 0 0 0	

2249. $C_{10}H_{16}N_2O_4$

Methyl-2,2-diallylmalonurate
Methyl 2,2-diallylmalonurate

RN: 73632-82-3 **MP** (°C)**:** 84
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.552E+00	23	B152	1 2 1 1 1	pH 3.5

2250. $C_{10}H_{16}N_4O_2$

7-Butyl theophylline
1H-Purine-2,6-dione, 7-butyl-3,7-dihydro-1,3-dimethyl-
7-Butyl-1,3-dimethylxanthine

RN: 1021-65-4 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	3.499E+00	30	B042	1 2 1 1 2	
1.560E-02	3.499E+00	30	G021	1 0 0 0 2	

2251. $C_{10}H_{16}N_4O_2S$

3-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-4-hydroxy-1
2-Imidazolidinone, 3-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-4-hydroxy-1-methyl-
Buthidazole
Ravage
VEL 5026

RN: 55511-98-3 **MP** (°C)**:** 133.5
MW: 256.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.322E-02	3.388E+00	25	M161	1 0 0 0 1	

2252. $C_{10}H_{16}N_6S$

Cimetidine
2-Cyano-1-methyl-3-(2-(((5-methylimidazol-4-yl)methyl)thio)ethyl)guanidine
N″-Cyano-*N*-methyl-*N′*-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine
N″-Cyano-*N*-methyl-*N′*-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine
Sigmetadine
Peptol

RN: 51481-61-9 **MP** (°C)**:** 142
MW: 252.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	6.010E+00	22.5	B422	2 0 2 2 2	
3.685E-02	9.300E+00	25	A412	1 0 2 2 1	int
3.963E-03	1.000E+00	ns	K444	0 0 0 0 0	

2253. $C_{10}H_{16}O$

D-Fenchone
D-1,3,3-Trimethyl-2-norbornanone
Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1*S*)-
α-Fenchone
(+)-Fenchone

RN: 4695-62-9 **MP** (°C)**:** 6.1
MW: 152.24 **BP** (°C)**:** 193.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-02	1.996E+00	20	D052	1 1 0 0 0	
1.410E-02	2.147E+00	25	I019	1 0 1 2 2	
1.413E-02	2.150E+00	ns	S460	0 0 0 0 0	

2254. $C_{10}H_{16}O$
D-Camphor
D-Campher
Camphor
RN: 76-22-2 **MP** (°C)**:** 179.7
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	1.667E+00	15.50	L073	1 2 2 1 2	
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	
1.363E-02	2.076E+00	20	K078	1 0 2 1 2	
1.030E-02	1.568E+00	25	I019	1 0 1 2 2	
1.340E-02	2.040E+00	25	L338	1 0 1 1 2	
1.630E-02	2.481E+00	37	E028	1 0 1 1 2	
1.115E-02	1.697E+00	ns	F014	0 0 0 0 2	
1.023E-02	1.558E+00	ns	R427	0 0 0 0 0	

2255. $C_{10}H_{16}O$
Carvotan acetone
Carvotan-aceton
RN: 499-71-8 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.912E-03	9.000E-01	20	F300	1 0 0 0 0	

2256. $C_{10}H_{16}O$
Citral
trans-3,7-dimethyl-2,6-octadienal
Geranialdehyde
Neral
Geranial
Citral A
RN: 5392-40-5 **MP** (°C)**:** <10
MW: 152.24 **BP** (°C)**:** 92.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	5.785E-01	25	A401	1 0 2 2 0	
1.583E-03	2.410E-01	25	L450	0 0 0 0 0	
1.970E-03	2.999E-01	25	M350	1 0 1 1 1	
8.800E-03	1.340E+00	37	E028	1 0 1 1 1	
8.710E-03	1.326E+00	ns	S460	0 0 0 0 0	

2257. $C_{10}H_{16}O$
L-Dihydrocarvone
L-Dihydro-carvon
RN: 619-02-3 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:** 221

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	

2258. $C_{10}H_{16}O$
Neral
RN: 106-26-3 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.898E-03	2.890E-01	25	L450	0 0 0 0 0	

2259. $C_{10}H_{16}O_2$
3-Hydroxy-3-ethynyl-2,2,5,5-tetramethyltetrahydrofuran
3-Furanol, 3-ethynyltetrahydro-2,2,5,5-tetramethyl-
RN: 24270-82-4 **MP** (°C)**:**
MW: 168.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.165E-01	1.961E+01	rt	B066	0 2 0 0 0	

2260. $C_{10}H_{16}O_3$
cis-Pinonic acid
cis-3-Acetyl-2,2-dimethylcyclobutaneacetic acid
RN: 473-72-3 **MP** (°C)**:** 104–107
MW: 184.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.001E-02	3.686E+00	0	H430	0 0 0 0 0	
3.612E-02	6.655E+00	rt	H431	0 0 0 0 0	average

2261. $C_{10}H_{16}O_4$
L-Isocamphoric acid
L-Isocamphersaeure
RN: 5394-83-2 **MP** (°C)**:** 173
MW: 200.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.698E-02	3.400E+00	20	F300	1 0 0 0 1	

2262. $C_{10}H_{16}O_4$

D-Camphoric acid
D-Camphersaeure
RN: 124-83-4 **MP** (°C)**:**
MW: 200.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.796E-02	7.600E+00	25	F300	1 0 0 0 1	

2263. $C_{10}H_{16}O_5$

DL-Cineolic acid
DL-Cineolsaeure
RN: 473-18-7 **MP** (°C)**:** 208
MW: 216.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-02	1.400E+01	15	F300	1 0 0 0 1	
3.006E-01	6.500E+01	100	F300	1 0 0 0 1	

2264. $C_{10}H_{17}Cl_2NOS$

Diallate
DATC
S-(2,3-Dichloroallyl-*N,N*-diisopropylthiocarbamate
RN: 2303-16-4 **MP** (°C)**:** –10
MW: 270.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	4.000E-02	25	B185	0 0 0 0 0	
5.181E-05	1.400E-02	25	B200	1 0 0 1 1	
1.480E-04	4.000E-02	25	M061	1 0 0 0 1	
5.181E-05	1.400E-02	25	M161	1 0 0 0 1	
1.480E-04	4.000E-02	ns	F019	0 0 0 0 1	
1.480E-04	4.000E-02	rt	I314	0 0 0 0 0	

2265. $C_{10}H_{17}NO_2$

Methyprylon
Dimerin
3,3-Diethyl-5-methyl-2,4-piperidinedione
RN: 125-64-4 **MP** (°C)**:**
MW: 183.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.147E-01	7.600E+01	25	R027	0 0 0 0 0	

2266. $C_{10}H_{17}N_2O_4PS$
Etrimfos
Dimethyl *O*-(2-ethyl-4-ethoxy-pyrimidin-6-yl)thionophosphate
Ekamet G
Ekamet ULV
Etrimphos
RN: 38260-54-7 **MP** (°C)**:**
MW: 292.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.421E-02	1.000E+01	20	M161	1 0 0 0 1	
1.368E-04	3.998E-02	ns	S460	0 0 0 0 0	

2267. $C_{10}H_{17}N_3O_5$
Orotic acid choline
RN: **MP** (°C)**:** 102–104
MW: 259.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.697E+00	6.992E+02	25	N018	0 0 0 0 0	

2268. $C_{10}H_{17}N_3O_6S$
Glutathione
Glutathion
RN: 70-18-8 **MP** (°C)**:** 193.4
MW: 307.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.958E-01	9.090E+01	0	F300	1 0 0 0 2	

2269. $C_{10}H_{17}O_3P$
Diethyl phenyl phosphonate
Diethyl benzenephosphonate
Diethyl phenylphosphonate
RN: 1754-49-0 **MP** (°C)**:**
MW: 216.22 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.25E-04	<2.00E-01	25	B070	1 2 0 1 0	

2270. $C_{10}H_{18}$
2,2,5,5-Tetramethyl-3-hexyne
Di-*tert*-butylacetylene
Di-*tert*-butylethyne
RN: 17530-24-4 **MP** (°C)**:**
MW: 138.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-04	2.032E-02	25	H039	1 2 2 2 2	
7.700E-05	1.065E-02	35	H039	1 2 2 2 1	

2271. $C_{10}H_{18}$
Pinane
2,6,6-Trimethylbicyclo[3.1.1]heptane
2,7,7-Trimethylbicyclo[3.1.1]heptane
Dihydropinene
RN: 473-55-2 **MP** (°C)**:**
MW: 138.25 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-05	1.576E-03	ns	S460	0 0 0 0 0	

2272. $C_{10}H_{18}$
Decalin
Decahydronaphthalene
RN: 91-17-8 **MP** (°C)**:** –31
MW: 138.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.45E-03	<2.00E-01	25	B019	1 0 1 2 0	
6.430E-06	8.890E-04	25	P051	2 1 1 2 2	
6.148E-06	8.500E-04	25	T423	0 0 0 0 0	
6.430E-06	8.890E-04	25.00	P007	2 1 2 2 2	
4.492E-05	6.210E-03	ns	H123	0 0 0 0 0	

2273. $C_{10}H_{18}$
cis-Decalin
cis-Decahydronaphthalene
cis-Bicyclo[4.4.0]decane
RN: 493-01-6 **MP** (°C)**:** –43.2
MW: 138.25 **BP** (°C)**:** 195.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.452E-02	8.920E+00	300	S355	1 1 1 2 0	EFG

2274. $C_{10}H_{18}ClN_5$
Ipazine
2-Chloro-4-diethylamino-6-isopropylamino-*s*-triazine
2-Chloro-4-isopropylamino-6-biethylamino-*s*-triazines
RN: 1912-25-0 **MP** (°C)**:**
MW: 243.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	4.000E-02	21	B192	0 0 0 0 1	
1.641E-04	4.000E-02	21	G099	2 0 0 1 0	
1.641E-04	4.000E-02	ns	B185	0 0 0 0 0	

2275. $C_{10}H_{18}N_2O_4$
Ethyl-2,2-diethylmalonurate
Ethyl 2,2-diethylmalnurate
RN: 73632-76-5 **MP** (°C)**:** 84.5
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-03	1.934E+00	23	B152	1 2 1 1 1	pH 3.5

2276. $C_{10}H_{18}N_2O_5$
Methoxymethyl-2,2-diethylmalonurate
Methoxymethyl 2,2-diethylmalonurate
RN: 73632-79-8 **MP** (°C)**:** 113
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.675E+00	23	B152	1 2 1 1 1	pH 3.5

2277. $C_{10}H_{18}N_6O_2$
1-(Sarcosino)-3,5-bis(dimethylamino)-*s*-triazine
*N*2-Carboxymethyl-*N*2,*N*4,*N*4,*N*6,*N*6-pentamethylmelamine
RN: 64124-17-0 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.360E-02	1.872E+01	25	B386	0 0 0 0 0	

2278. $C_{10}H_{18}O$
Borneol
endo-1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol
L-Borneol
RN: 507-70-0 **MP** (°C)**:** 206
MW: 154.25 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.512E-03	6.960E-01	15	M073	1 0 2 2 2	
4.784E-03	7.380E-01	25	M073	1 0 2 2 2	
4.786E-03	7.383E-01	ns	R427	0 0 0 0 0	

2279. $C_{10}H_{18}O$
D-Borneol
Borneocamphor
Sumatra camphor
endo-2-Bornanol
RN: 464-43-7 **MP** (°C)**:** 208
MW: 154.25 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-03	7.400E-01	25	F300	1 0 0 0 1	

2280. $C_{10}H_{18}O$
L-Menthone
trans-p-Menthan-3-one
p-Menthan-3-one
(–)-5-Methyl-2-(1-methylethyl)cyclohexanone
(–)-Menthone
RN: 14073-97-3 **MP** (°C)**:** –6
MW: 154.25 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.220E-03	4.967E-01	25	I019	1 0 1 2 2	

2281. $C_{10}H_{18}O$
Linalool
3,7-Dimethylocta-1,6-dien-3-ol
2,6-Dimethylocta-2,7-dien-6-ol
Linalol
3,7-Dimethyl-1,6-octadien-3-ol
RN: 78-70-6 **MP** (°C)**:** <25
MW: 154.25 **BP** (°C)**:** 195.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.507E-01	6	P430	0 0 0 0 0	
5.530E-03	8.530E-01	23.5	P430	0 0 0 0 0	
1.200E-02	1.851E+00	25	D407	1 0 2 2 2	
1.030E-02	1.589E+00	25	I019	1 0 1 2 2	
9.710E-03	1.498E+00	25	M350	1 0 1 1 1	
3.800E-02	5.862E+00	37	E028	1 0 1 1 2	

2282. $C_{10}H_{18}O$
Citronellal
D-Citronellal
(*R*)-(+)-citronellal
3,7-Dimethyl-6-octen-1-al
3,7-Dimethyl-6-octenal
Rhodinal
RN: 106-23-0 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	1.388E-01	25	A401	1 0 2 2 0	

2283. $C_{10}H_{18}O$
α-Terpineol
1-*p*-Menthen-8-ol
1-Methyl-4-isopropyl-1-cyclohexen-8-ol
2-(4-Methyl-3-cyclohexenyl)-2-propanol
p-Menth-1-en-8-ol
α,α,4-Trimethyl-3-cyclohexene-1-methanol
RN: 98-55-5 **MP** (°C)**:** 34.5
MW: 154.25 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.202E-03	3.397E-01	6	P430	0 0 0 0 0	
4.600E-03	7.096E-01	23.5	P430	0 0 0 0 0	
1.620E-02	2.499E+00	25	A401	1 0 2 2 0	

2284. $C_{10}H_{18}O$
Nerol
Allerol
cis-3,7-Dimethyl-2,6-octadien-1-ol
Neraniol
Nerosol
Vernol
RN: 106-25-2 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	1.311E+00	25	A401	1 0 2 2 0	

2285. $C_{10}H_{18}O$
Geraniol
2,6-Dimethyl-2,6-octadien-8-ol
2,6-Dimethyl-*trans*-2,6-octadien-8-ol
2-*trans*-3,7-Dimethyl-2,6-octadiene-1-ol
3,7-Dimethyl-*trans*-2,6-octadien-1-ol
(E)-3,7-Dimethyl-2,6-octadien-1-ol
RN: 106-24-1 **MP** (°C)**:** 15
MW: 154.25 **BP** (°C)**:** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	7.713E-01	25	A401	1 0 2 2 0	

2286. $C_{10}H_{18}O$
Menthone
5-Methyl-2-(1-methylethyl)cyclohexanone
DL-Menthone
RN: 10458-14-7 **MP** (°C)**:** –6
MW: 154.25 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.085E-01	25	A401	1 0 2 2 0	

2287. $C_{10}H_{18}O$
Plinol
RN: 72402-00-7 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.281E-03	8.146E-01	6	P430	0 0 0 0 0	
9.610E-03	1.482E+00	23.5	P430	0 0 0 0 0	

2288. $C_{10}H_{18}O$
1,8-Cineole
Eucalyptol
Cineol
Cineole
RN: 470-82-6 **MP** (°C)**:** 36.5
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.123E-02	6.359E+00	1.5	E036	1 0 1 1 1	
4.187E-02	6.458E+00	4.0	B352	0 0 0 0 0	
3.674E-02	5.668E+00	7.5	E036	1 0 1 1 1	
3.482E-02	5.371E+00	10	E036	1 0 1 1 1	
3.610E-02	5.569E+00	10.0	B352	0 0 0 0 0	
1.297E-02	2.000E+00	15	F300	1 0 0 0 1	
3.097E-02	4.777E+00	15.0	B352	0 0 0 0 0	
2.261E-02	3.488E+00	21	E036	1 0 1 1 1	
2.454E-02	3.786E+00	21.0	B352	0 0 0 0 0	
2.010E-02	3.100E+00	25	A049	1 0 0 0 1	
2.197E-02	3.388E+00	25	B423	1 1 1 2 1	
1.746E-02	2.693E+00	30.0	B352	0 0 0 0 0	
1.552E-02	2.394E+00	35.0	B352	0 0 0 0 0	
9.100E-03	1.404E+00	37	E028	1 0 1 1 1	
1.359E-02	2.096E+00	40	E036	1 0 1 1 1	
1.423E-02	2.195E+00	40.0	B352	0 0 0 0 0	
1.294E-02	1.996E+00	45.0	B352	0 0 0 0 0	
1.229E-02	1.896E+00	50	E036	1 0 1 1 1	
1.100E-02	1.697E+00	50.0	B352	0 0 0 0 0	

2289. $C_{10}H_{18}O_2$
2,4-Decadione
Acetylmethyl hexyl ketone
RN: 13329-78-7 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.427E-01	25	M078	2 0 1 0 1	

2290. $C_{10}H_{18}O_2$
3-Pentyl-2,4-pentadione
3-Amyl-2,4-pentanedione
RN: 27970-50-9 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	2.401E+00	25	M078	2 0 1 0 2	

2291. $C_{10}H_{18}O_2$
Sobrerol
Pinolhydrat
RN: 498-71-5 **MP** (°C)**:** 130
MW: 170.25 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-01	3.200E+01	15	F300	1 0 0 0 1	
1.938E-01	3.300E+01	ns	L335	0 0 0 0 2	

2292. $C_{10}H_{18}O_2$
D-Campholic acid
D-Campholsaeure
RN: 464-88-0 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.398E-04	1.600E-01	19	F300	1 0 0 0 1	

2293. $C_{10}H_{18}O_3$
2,2,5,5-Tetramethyl-tetrahydro-3-hydroxy-3-furanyl methyl ketone
Ketone, methyl tetrahydro-3-hydroxy-2,2,5,5-tetramethyl-3-furyl
RN: 24282-51-7 **MP** (°C)**:**
MW: 186.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2294. $C_{10}H_{18}O_4$
Sebacic acid
Sebacinsaeure
RN: 111-20-6 **MP** (°C)**:** 134.5
MW: 202.25 **BP** (°C)**:** 294.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-04	4.000E-02	0	F300	1 0 0 0 0	
1.978E-04	4.000E-02	0	L041	1 0 0 1 0	
4.944E-03	1.000E+00	20	F300	1 0 0 0 1	
4.944E-03	1.000E+00	20	L041	1 0 0 1 1	
9.889E-03	2.000E+00	21	B040	1 0 1 1 1	*sic*
7.911E-03	1.600E+00	35	L041	1 0 0 1 1	
1.088E-02	2.200E+00	50	L041	1 0 0 1 1	
2.077E-02	4.200E+00	65	F300	1 0 0 0 1	
2.077E-02	4.200E+00	65	L041	1 0 0 1 1	
8.898E-04	1.800E-01	ns	F014	0 0 0 0 1	

2295. $C_{10}H_{18}O_4$
Amyl α-acetoxypropionate
Hydracrylic acid, pentyl ester, acetate
RN: 20473-77-2 **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.461E-03	7.000E-01	25	R006	2 2 0 1 1	

2296. $C_{10}H_{18}O_4$
Ethylene glycol dibutyrate
Ethylene glycol di-*N*-butyrate
RN: 105-72-6 **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-03	1.663E+00	25	F064	1 0 0 0 2	
2.471E-03	4.998E-01	ns	F014	0 0 0 0 1	

2297. $C_{10}H_{18}O_4$
Diethoxyethyl adipate
Diethyl adipate
RN: 141-28-6 **MP** (°C)**:** –18
MW: 202.25 **BP** (°C)**:** 251

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.965E-03	5.996E-01	ns	F014	0 0 0 0 1	
1.223E-02	2.474E+00	ns	F014	0 0 0 0 2	

2298. $C_{10}H_{18}O_4$
Dimethyl cyclohexyl oxalate
RN: **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.89E-06	<2.00E-03	15	H069	1 0 1 1 0	

2299. $C_{10}H_{18}O_5$
Diethylene glycol dipropionate
Ethanol, 2,2′-oxybis-, dipropanoate
RN: 6942-59-2 **MP** (°C)**:**
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.592E-01	3.475E+01	ns	F014	0 0 0 0 2	

2300. $C_{10}H_{18}O_5$
Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, butyl ester
Propanoic acid, 2-[(amoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.290E-03	4.998E-01	25	R007	0 0 0 0 0	
3.205E-03	6.995E-01	25	R007	0 0 0 0 0	

2301. $C_{10}H_{19}NO_2S$
4-Thiazolidinecarboxylic acid, 2-hexyl-
Thiazolidine-4-carboxylic acid, 2-hexyl-
RN: 14347-74-1 **MP** (°C)**:**
MW: 217.33 **BP** (°C)**:** 378.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.085E-01	21	B414	1 0 0 1 1	partial decomposition

2302. $C_{10}H_{19}NO_3$
Ethylpropylaceturethane
RN: **MP** (°C)**:**
MW: 201.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.088E-03	1.427E+00	c	O021	0 2 0 0 0	

2303. $C_{10}H_{19}NO_3$
Oenanthylylurethane
RN: **MP** (°C)**:**
MW: 201.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.043E-03	2.100E-01	ns	O021	0 0 0 0 0	

2304. $C_{10}H_{19}NO_4S$
2-Amino-5-naphthol-1-sulfonic acid
RN: **MP** (°C)**:**
MW: 249.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.503E-03	2.120E+00	c	B125	1 2 0 0 2	

2305. $C_{10}H_{19}N_2O_4PS$

Cyanthoate
Phosphorothioic acid, *S*-(2-((1-cyano-1-methylethyl)amino)-2-oxoethyl) *O,O*-diethyl ester
Tartran
RN: 3734-95-0 **MP** (°C)**:**
MW: 294.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	7.000E+01	20	M161	1 0 0 0 1	

2306. $C_{10}H_{19}N_5O$

Prometone
2-Methoxy-4,6-*bis*-isopropylamino-*s*-triazine
Pramitol
Primatol O
Prometon
2-Methoxy-4,6-*bis*-(isopropyl-amino)-*s*-triazine
RN: 1610-18-0 **MP** (°C)**:** 91.5
MW: 225.30 **BP** (°C)**:** 91–92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.330E-03	7.502E-01	20	B200	1 0 0 0 2	
2.752E-03	6.200E-01	20	F311	1 2 2 2 1	
3.329E-03	7.500E-01	20	M161	1 0 0 0 2	
3.329E-03	7.500E-01	21	B192	0 0 0 0 2	
1.554E-02	3.500E+00	21	G099	2 0 0 1 0	
3.329E-03	7.500E-01	21	G099	2 0 0 1 0	
4.680E-03	1.054E+00	50	G001	1 0 1 1 2	
3.548E-03	7.994E-01	ns	B100	0 0 0 0 0	
3.329E-03	7.500E-01	ns	B185	0 0 0 0 0	
3.329E-03	7.500E-01	ns	C101	0 0 0 0 1	
3.329E-03	7.500E-01	ns	G041	0 0 0 0 2	
3.329E-03	7.500E-01	ns	H112	0 0 0 0 2	
3.329E-03	7.500E-01	ns	J033	0 0 0 0 0	

2307. $C_{10}H_{19}N_5O$

Terebumeton
1,3,5-Triazine-2,4-diamine, *N*-(1,1-dimethylethyl)-*N′*-ethyl-6-methoxy-
2-Methoxy-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Karagard
4-(Ethylamino)-2-methoxy-6-(*tert*-butylamino)-*s*-triazine
Caragard
RN: 33693-04-8 **MP** (°C)**:** 123.5
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.770E-04	1.300E-01	20	M161	1 0 0 0 2	

2308. $C_{10}H_{19}N_5O$
2-Methoxy-4-ethylamino-6-diethylamino-*s*-triazine
G 31432
RN: 13532-26-8 **MP** (°C)**:**
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-04	4.000E-02	20	J033	0 0 0 0 0	

2309. $C_{10}H_{19}N_5O$
Secbumeton
2-*sec*-Butylamino-4-ethylamino-6-methoxy-*s*-triazine
GS-14254
RN: 26259-45-0 **MP** (°C)**:** 86
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.930E-03	6.601E-01	1	G091	1 0 1 2 2	pH 6.0
3.250E-03	7.322E-01	8	G091	1 0 1 2 2	pH 6.0
2.750E-03	6.196E-01	20	B200	1 0 0 0 2	
2.663E-03	6.000E-01	20	F311	1 2 2 2 1	
3.070E-03	6.917E-01	20	G091	1 0 1 2 2	pH 6.0
2.752E-03	6.200E-01	20	M161	1 0 0 0 2	
3.300E-03	7.435E-01	29	G091	1 0 1 2 2	pH 6.0

2310. $C_{10}H_{19}N_5OS$
Hydroxyprometryne
1,3,5-Triazin-2(1H)-one, 4,6-bis[(1-methylethyl)amino]-
bis(Isopropylamino)hydroxy-*s*-triazine
GS 11526
RN: 7374-53-0 **MP** (°C)**:**
MW: 257.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.029E-01	2	B193	1 2 0 0 0	

2311. $C_{10}H_{19}N_5S$
Terbutryn
2-Methylthio-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Terbutryne
N-(1,1-Dimethylethyl)-*N′*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Terbutrex
RN: 886-50-0 **MP** (°C)**:** 104
MW: 241.36 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	2.631E-02	1	G091	1 0 1 2 2	pH 6.0
1.100E-04	2.655E-02	8	G091	1 0 1 2 2	pH 6.0
2.400E-04	5.793E-02	20	B200	1 0 0 0 1	
1.036E-04	2.500E-02	20	E048	1 2 1 1 1	
1.036E-04	2.500E-02	20	F311	1 2 2 2 1	
1.460E-04	3.524E-02	20	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	20	M161	1 0 0 0 1	
1.660E-04	4.007E-02	29	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	ns	J033	0 0 0 0 0	

2312. $C_{10}H_{19}N_5S$
Prometryne
N,N′-bis(1-Methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine
Caparol
Primatol Q
Gesagard
Caparol 80W
RN: 7287-19-6 **MP** (°C)**:** 118
MW: 241.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.793E-02	2	B193	1 2 0 0 0	
2.000E-04	4.827E-02	20	B200	1 0 0 0 0	
1.657E-04	4.000E-02	20	F311	1 2 2 2 1	
1.988E-03	4.798E-01	20	M061	1 0 0 0 1	
1.989E-04	4.800E-02	20	M161	1 0 0 0 1	
1.989E-04	4.800E-02	24	C105	2 1 2 2 2	
4.200E-04	1.014E-01	50	G001	1 0 1 1 2	
1.989E-04	4.800E-02	ns	C101	0 0 0 0 1	
1.989E-04	4.800E-02	ns	H112	0 0 0 0 1	
1.989E-04	4.800E-02	ns	J033	0 0 0 0 0	

2313. $C_{10}H_{19}N_5S$
s-Triazole, 2,4-bis(isopropylamine)-6-methylmercapto-
RN: **MP** (°C)**:**
MW: 241.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E-04	4.800E-02	20	B185	0 0 0 0 0	

2314. $C_{10}H_{19}O_6PS_2$
Malathion
Dicarboethoxyethyl *O,O*-dimethyl phosphorodithioate
Carbofos
Cythion
Mercaptothion
Phosphothion
RN: 121-75-5 **MP** (°C)**:** 3
MW: 330.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.267E-04	1.410E-01	10	B324	0 0 0 0 0	
4.268E-04	1.410E-01	10	B324	0 0 0 0 0	
4.329E-04	1.430E-01	20	B300	2 1 1 1 2	
4.389E-04	1.450E-01	20	B324	0 0 0 0 0	
4.388E-04	1.450E-01	20	B324	0 0 0 0 0	
4.389E-04	1.450E-01	20	F311	1 2 2 2 1	
4.389E-04	1.450E-01	20	M061	1 0 0 0 2	
4.389E-04	1.450E-01	20	M344	1 0 0 0 2	
4.964E-04	1.640E-01	30	B324	0 0 0 0 0	
4.963E-04	1.640E-01	30	B324	0 0 0 0 0	
4.389E-04	1.450E-01	rt	M161	0 0 0 0 2	

2315. $C_{10}H_{20}$
Cyclodecane
RN: 293-96-9 **MP** (°C)**:** 10
MW: 140.27 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-06	3.300E-04	25	T423	0 0 0 0 0	

2316. $C_{10}H_{20}$
n-Pentylcyclopentane
1-Pentylcyclopentane
RN: 3741-00-2 **MP** (°C)**:**
MW: 140.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.198E-07	1.150E-04	25	K119	1 0 0 0 2	
8.198E-07	1.150E-04	25	P051	2 1 1 2 2	
8.198E-07	1.150E-04	25.00	P007	2 1 2 2 2	

2317. $C_{10}H_{20}NO_4PS$
Propetamphos
Methylethyl (E)-3-(((ethylamino)methoxyphosphinothioyl)oxy)-2-butenoate
Safrotin
Seraphos
Zoecon
RN: 31218-83-4 **MP** (°C)**:**
MW: 281.31 **BP** (°C)**:** 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-04	1.100E-01	24	M161	1 0 0 0 2	

2318. $C_{10}H_{20}NO_5PS_2$
Mecarbam
O,O-Diethyl *S*-(*N*-methyl-*N*-carboethoxycarbamoylmethyl) dithiophosphate
RN: 2595-54-2 **MP** (°C)**:**
MW: 329.38 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.033E-03	9.990E-01	rt	M061	0 0 0 0 0	
<3.04E-03	<1.00E+00	rt	M161	0 0 0 0 0	

2319. $C_{10}H_{20}N_2S_4$
Disulfiram
Tetraethylthioperoxydicarbonothioic diamide
Tetraethylthiuram disulfide
Antadix
Antabuse
Esperal
RN: 97-77-8 **MP** (°C)**:** 70
MW: 296.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.744E-04	2.000E-01	25	I314	0 0 0 0 0	
1.379E-05	4.090E-03	25	L033	1 0 2 1 2	*sic*
1.012E-03	3.000E-01	ns	N061	0 0 0 0 0	

2320. $C_{10}H_{20}N_6O$
N-(Methoxymethyl)pentamethylmelamine
N-Methylolpentamethylmelamine methyl ether
RN: 64124-15-8 **MP** (°C)**:** 39
MW: 240.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-03	1.500E+00	25	C051	1 2 1 1 1	pH 7, unstable in water

2321. $C_{10}H_{20}O$
Citronellol
3,7-Dimethyl-6-octen-1-ol
Levo-citronellol
β-Citronellol
RN: 106-22-9 **MP** (°C)**:**
MW: 156.27 **BP** (°C)**:** 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-03	2.000E-01	25	M350	1 0 1 1 1	

2322. $C_{10}H_{20}O$
Decanal
Cuprylaldehyde
RN: 112-31-2 **MP** (°C)**:** 7
MW: 156.27 **BP** (°C)**:** 207–209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.983E-05	1.560E-02	25	L450	0 0 0 0 0	

2323. $C_{10}H_{20}O$
Menthol
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-
3-*p*-Menthanol
RN: 89-78-1 **MP** (°C)**:** 42
MW: 156.27 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-03	4.000E-01	20	F300	1 0 0 0 2	
2.920E-03	4.563E-01	25	I019	1 0 1 2 2	
8.600E-03	1.344E+00	37	E028	1 0 1 1 1	

2324. $C_{10}H_{20}O$
l-Menthol
1-Isopropyl-4-methyl cyclohexan-2-ol
1-Methyl-4-isopropyl cyclohexan-3-ol
(1R,2S,5R)-(–)-Menthol
5-Methyl-2-isopropyl hexahydrophenol
Cyclohexanol
RN: 2216-51-5 **MP** (°C)**:** 44
MW: 156.27 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	6.251E-01	25	A401	1 0 2 2 0	

2325. $C_{10}H_{20}O_2$
3-Hydroxy-2-ethyl-5-propyl-5-methyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5-methyl-5-propyl-
RN: 29839-73-4 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2326. $C_{10}H_{20}O_2$
3-Hydroxy-2,2-dimethyl-5,5-diethyltetrahydrofuran
3-Furanol, 5,5-diethyltetrahydro-2,2-dimethyl-
RN: 29839-77-8 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2327. $C_{10}H_{20}O_2$
3-Hydroxy-2,5,5-triethyltetrahydrofuran
3-Furanol, 2,5,5-triethyltetrahydro-
RN: 29839-70-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2328. $C_{10}H_{20}O_2$
3-Hydroxy-2,5-dipropyltetrahydrofuran
3-Furanol, 2,5-dipropyltetrahydro-
RN: 30003-27-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2329. $C_{10}H_{20}O_2$
3-Hydroxy-2-butyl-5,5-methyltetrahydrofuran
3-Furanol, 2-butyltetrahydro-5,5-dimethyl-
RN: 29839-71-2 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2330. $C_{10}H_{20}O_2$
3-Hydroxy-2-pentyl-5-methyltetrahydrofuran
3-Furanol, 5-methyltetrahydro-2-pentyl-
RN: 29848-45-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2331. $C_{10}H_{20}O_2$
3-Hydroxy-2-propyl-5-methyl-5-ethyltetrahydrofuran
3-Furanol, 5-ethyltetrahydro-5-methyl-2-propyl-
RN: 29839-72-3 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2332. $C_{10}H_{20}O_2$
n-Capric acid
Caprinsaeure
Decanoic acid
Nonanecarboxylic acid
RN: 334-48-5 **MP** (°C)**:** 31.4
MW: 172.27 **BP** (°C)**:** 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.515E-04	9.500E-02	0	B136	1 0 2 1 1	
1.509E-04	2.600E-02	15	F300	1 0 0 0 1	
2.902E-04	5.000E-02	20	A011	1 2 1 1 1	
9.462E-04	1.630E-01	20	B136	1 0 2 1 2	
8.706E-04	1.500E-01	20	D041	1 0 0 0 1	
8.706E-04	1.500E-01	20.0	R001	1 1 1 1 1	
3.590E-04	6.184E-02	25	J001	1 0 2 1 2	
1.115E-03	1.920E-01	30	B136	1 0 2 1 2	
3.715E-04	6.400E-02	30	E005	2 1 1 2 1	
1.045E-03	1.800E-01	30.0	R001	1 1 1 1 1	
1.294E-03	2.230E-01	40	B136	1 0 2 1 2	
4.179E-04	7.200E-02	40	E005	2 1 1 2 1	
1.335E-03	2.300E-01	45	B136	1 0 2 1 1	
1.335E-03	2.299E-01	45.0	R001	1 1 1 1 1	
4.702E-04	8.100E-02	50	E005	2 1 1 2 1	
5.000E-04	8.613E-02	50	J001	1 0 2 1 2	
1.567E-03	2.700E-01	60	B136	1 0 2 1 1	
5.805E-04	1.000E-01	60	E005	2 1 1 2 2	
1.567E-03	2.699E-01	60.0	R001	1 1 1 1 1	
5.514E-04	9.499E-02	.0	R001	1 1 1 1 1	

2333. $C_{10}H_{20}O_2$
3-Hydroxy-5,5-dipropyltetrahydrofuran
3-Furanol, 5,5-dipropyltetrahydro-
RN: 29839-54-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2334. $C_{10}H_{20}O_2$
3-Hydroxy-5,5-diisopropyltetrahydrofuran
3-Furanol, 5,5-diisopropyltetrahydro-
RN: 29839-55-2 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2335. $C_{10}H_{20}O_2$
3-Hydroxy-2,5-dimethyl-2,5-diethyltetrahydrofuran
3-Furanol, 2,5-diethyltetrahydro-2,5-dimethyl-
RN: 30010-09-4 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-01	1.961E+01	rt	B066	0 2 0 0 0	

2336. $C_{10}H_{20}O_2.H_2O$
Terpin (monohydrate)
Terpin-hydrat
RN: 2451-01-6 **MP** (°C)**:** 116
MW: 190.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.102E-02	4.000E+00	15	F300	1 0 0 0 0	
1.799E-02	3.424E+00	25	M012	1 0 2 1 2	
1.661E-01	3.160E+01	100	F300	1 0 0 0 2	

2337. $C_{10}H_{20}O_3$
1,3-Dioxolane-4-methanol, 2-methyl-2-pentyl
2-Heptanone, cyclic (hydroxymethyl)ethylene acetal
2-Methyl-2-*n*-amyl-4-hydroxymethyl-1,3-dioxolane
2-Methyl-2-pentyl-1,3-dioxolane-4-methanol
RN: 4361-59-5 **MP** (°C)**:**
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.090E-02	9.583E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2338. $C_{10}H_{20}O_3$
n-Amyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, pentyl ester
RN: 14144-36-6 **MP** (°C)**:**
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.366E-03	1.199E+00	25	D002	1 2 1 1 1	

2339. $C_{10}H_{20}O_4$
Butyl carbitol acetate
Diethylene glycol acetate butyl ether
Diethylene glycol butyl ether acetate
Diglykol-monobutylaether-acetat
RN: 124-17-4 **MP** (°C)**:** –32
MW: 204.27 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.709E-02	1.575E+01	20	D052	1 1 0 0 1	
1.792E-01	3.661E+01	20	M062	1 0 0 0 1	

2340. $C_{10}H_{21}NOS$
Pebulate
S-Propyl butylethylthiocarbamate
RN: 1114-71-2 **MP** (°C)**:** <25
MW: 203.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-04	6.000E-02	20	M161	1 0 0 0 1	
4.524E-04	9.200E-02	21	F019	1 0 0 0 1	
4.524E-04	9.200E-02	21	M061	1 0 0 0 1	
2.951E-04	6.000E-02	ns	B200	0 0 0 0 1	
2.951E-04	6.001E-02	ns	S460	0 0 0 0 0	

2341. $C_{10}H_{21}NOS$
Vernolate
S-Propyl dipropylthiocarbamate
Carbamic acid, dipropylthio-, *S*-propyl ester
Carbamate, *n*-propyl-di-*n*-propylthio-
Vernam
RN: 1929-77-7 **MP** (°C)**:** <25
MW: 203.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.426E-04	9.000E-02	20	B200	1 0 0 0 1	
5.262E-04	1.070E-01	21	F019	1 0 0 0 2	
5.262E-04	1.070E-01	21	M161	1 0 0 0 2	
<4.92E-04	<1.00E-01	ns	B185	0 0 0 0 0	
4.917E-04	9.999E-02	ns	M061	0 0 0 0 0	

2342. $C_{10}H_{22}$
2,2-Dimethyloctane
RN: 15869-87-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-07	1.067E-04	ns	S460	0 0 0 0 0	

2343. $C_{10}H_{22}$
n-Decane
Decane
Decyl hydride
RN: 124-18-5 **MP** (°C)**:** –30.0
MW: 142.29 **BP** (°C)**:** 174.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-07	1.976E-05	20	B165	1 0 1 1 1	
1.124E-07	1.600E-05	25	B069	1 0 1 1 1	
1.389E-07	1.976E-05	25	F004	0 0 0 0 0	
3.655E-07	5.200E-05	25	M003	1 0 2 2 1	
3.655E-07	5.200E-05	25	M040	1 0 0 1 1	
3.233E-07	4.600E-05	25	T423	0 0 0 0 0	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 2	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 0	
3.655E-07	5.200E-05	ns	H123	0 0 0 0 0	

2344. $C_{10}H_{22}$
4,4-Dimethyloctane
RN: 15869-95-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 157.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E-05	2.200E-03	20	M337	2 1 2 2 1	
7.278E-07	1.036E-04	ns	S460	0 0 0 0 0	

2345. $C_{10}H_{22}$
2,3-Dimethyloctane
RN: 7146-60-3 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.117E-07	7.281E-05	ns	S460	0 0 0 0 0	

2346. $C_{10}H_{22}$
2,6-Dimethyloctane
RN: 2051-30-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.266E-07	8.916E-05	ns	S460	0 0 0 0 0	

2347. $C_{10}H_{22}$
3,6-Dimethyloctane
RN: 15869-94-0 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.109E-07	8.693E-05	ns	S460	0 0 0 0 0	

2348. $C_{10}H_{22}$
3-Ethyloctane
RN: 5881-17-4 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-07	6.519E-05	ns	S460	0 0 0 0 0	

2349. $C_{10}H_{22}$
4-Methylnonane
4-Methylnonane(DL)
RN: 17301-94-9 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.764E-07	6.779E-05	ns	S460	0 0 0 0 0	

2350. $C_{10}H_{22}$
3,3-Dimethyloctane
RN: 4110-44-5 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.998E-07	8.534E-05	ns	S460	0 0 0 0 0	

2351. $C_{10}H_{22}$
4-Ethyloctane
RN: 15869-86-0 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.297E-07	7.536E-05	ns	S460	0 0 0 0 0	

2352. $C_{10}H_{22}$
3,5-Dimethyloctane
RN: 15869-93-9 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.546E-07	9.315E-05	ns	S460	0 0 0 0 0	

2353. $C_{10}H_{22}$
3-Methylnonane
3-Methylnonane(DL)
RN: 5911-04-6 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.295E-07	6.112E-05	ns	S460	0 0 0 0 0	

2354. $C_{10}H_{22}O$
Decanol
RN: 36729-58-5 **MP** (°C)**:**
MW: 158.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.166E-02	24	H345	0 0 0 0 0	

2355. $C_{10}H_{22}O$
n-Decyl alcohol
Alcohol C-10
Nonyl acarbinol
Capric alcohol
RN: 36729-58-5 **MP** (°C)**:**
MW: 158.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	4.258E-02	20	H330	0 0 0 0 0	
2.000E-04	3.166E-02	24	H345	2 0 2 2 2	
2.340E-04	3.704E-02	25	K025	2 2 1 1 2	
2.527E-05	4.000E-03	40	W305	1 0 0 1 0	EFG
3.000E-04	4.748E-02	ns	H012	0 2 2 0 0	

2356. $C_{10}H_{23}O_2PS_2$
Cadusafos
Ebufos
Taredan
Rugby
Apache
O-ethyl *S,S*-bis(1-methylpropyl) phosphorodithioate
RN: 95465-99-9 **MP** (°C)**:**
MW: 270.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.162E-04	2.477E-01	ns	S460	0 0 0 0 0	

2357. $C_{10}H_{23}O_3P$
Ethyl dibutyl phosphonate
Dibutyl ethyl phosphonate
RN: 2404-58-2 **MP** (°C)**:**
MW: 222.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.699E-02	6.000E+00	25	B070	1 2 0 1 0	
5.849E-02	1.300E+01	25	B070	1 2 0 1 1	

2358. $C_{10}H_{23}O_4P$
Dibutyl ethyl phosphate
RN: 7242-58-2 **MP** (°C)**:**
MW: 238.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-02	3.400E+00	25	B070	1 2 2 1 1	

2359. $C_{10}Cl_{10}O$

Chlordecone
Kepone
1,2,3,5,6,7,8,9,10,10-Decachloropentacyclo[5.2.1.0(2,6).0(3,9).0(5,8)]decano-4-one
Merex
Decachloroketone
RN: 143-50-0 **MP** (°C)**:**
MW: 490.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.153E-03	4.000E+00	100	M161	1 0 0 0 0	
6.166E-06	3.025E-03	ns	R424	0 0 0 0 0	
6.166E-06	3.025E-03	ns	R427	0 0 0 0 0	

2360. $C_{10}Cl_{12}$

Mirex
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene dimer
Bichlorendo
Ferriamicide
Dechlorane 4070
RN: 2385-85-5 **MP** (°C)**:**
MW: 545.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-07	8.450E-05	24.99	K436	0 0 0 0 0	
1.397E-10	7.619E-08	25	H434	0 0 0 0 0	
1.558E-07	8.500E-05	25	M134	1 2 1 1 1	
1.741E-07	9.500E-05	ns	M110	0 0 0 0 0	EFG
1.660E-07	9.054E-05	ns	R427	0 0 0 0 0	

2361. $C_{11}H_6BrNS$

1-Bromo-2-naphthylisothiocyanate
RN: 2392-80-5 **MP** (°C)**:**
MW: 264.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-05	1.268E-02	25	D019	1 1 1 1 1	

2362. $C_{11}H_6O_3$

Psoralen
7H-Furo[3,2-g][1]benzopyran-7-one
RN: 66-97-7 **MP** (°C)**:** 158–161
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-04	6.516E-02	25	A355	0 0 0 0 0	

2363. $C_{11}H_7Cl_2NO_3$
Pyoluteorin
RN: **MP** (°C)**:**
MW: 272.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.442E-01	5.0	L451	0 0 0 0 0	
5.600E-04	1.524E-01	10	L451	0 0 0 0 0	
6.300E-04	1.714E-01	15.0	L451	0 0 0 0 0	
7.500E-04	2.041E-01	20.0	L451	0 0 0 0 0	
7.900E-04	2.150E-01	25.0	L451	0 0 0 0 0	
9.600E-04	2.612E-01	30.0	L451	0 0 0 0 0	
9.900E-04	2.694E-01	35.0	L451	0 0 0 0 0	
1.150E-03	3.129E-01	40.0	L451	0 0 0 0 0	
1.290E-03	3.510E-01	45.0	L451	0 0 0 0 0	
1.500E-03	4.081E-01	50.0	L451	0 0 0 0 0	
1.590E-03	4.326E-01	55.0	L451	0 0 0 0 0	
1.730E-03	4.707E-01	60.0	L451	0 0 0 0 0	

2364. $C_{11}H_7FN_2O_3$
3-Benzoyl-5-fluorouracil
RN: 61251-77-2 **MP** (°C)**:** 169–170
MW: 234.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.551E-03	1.300E+00	22	B321	0 0 0 0 0	pH 4.0
5.551E-03	1.300E+00	22	B332	1 1 0 0 1	pH 4.0

2365. $C_{11}H_7FN_2O_4$
3-Phenyloxycarbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Phenyloxycarbonyl-5-fluorouracil
RN: 66999-97-1 **MP** (°C)**:** 169–170
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.995E-04	1.500E-01	22	B321	0 0 0 0 0	pH 4.0

2366. $C_{11}H_7FN_2O_4$
1-Phenyloxycarbonyl-5-fluorouracil
RN: 75410-28-5 **MP** (°C)**:**
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-03	9.000E-01	22	B332	1 1 0 0 1	pH 4.0

2367. $C_{11}H_7NS$
2-Naphthyl isothiocyanate
2-Isothiocyanatonaphthalene
β-Naphthyl mustard oil
RN: 1636-33-5 **MP** (°C)**:**
MW: 185.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	6.669E-03	25	D019	1 1 1 1 1	

2368. $C_{11}H_7NS$
1-Naphthyl isothiocyanate
1-Isothiocyanatonaphthalene
α-Naphthyl mustard oil
Kesscocide
ANI
ANIT
RN: 551-06-4 **MP** (°C)**:** 58.0
MW: 185.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	4.631E-03	25	D019	1 1 1 1 1	

2369. $C_{11}H_8N_2$
β-Carboline
β-Carbolin
Norharmane
9H-Pyrido(3,4-b)indole
RN: 244-63-3 **MP** (°C)**:** 199
MW: 168.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E+01	2.340E+03	16	B413	1 0 2 2 1	
1.601E+01	2.693E+03	17	B413	1 0 2 2 1	
2.535E+01	4.264E+03	37	B413	1 0 2 2 1	
2.561E+01	4.308E+03	38	B413	1 0 2 2 1	
2.916E+01	4.905E+03	45	B413	1 0 2 2 1	

2370. $C_{11}H_8N_4O_4$
Orotic acid nicotinmide
RN: **MP** (°C)**:** 252–253
MW: 260.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-02	1.769E+01	25	N018	0 0 0 0 0	

2371. $C_{11}H_8O_2$
2-Naphthoic acid
β-Naphthoic acid
2-Naphthalenecarboxylic acid
RN: 93-09-4 **MP** (°C)**:**
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.238E-02	25	M149	2 2 2 2 1	intrinsic, *sic*
1.617E-06	2.785E-04	30	K148	1 1 0 0 2	
2.323E-06	4.000E-04	40	K148	1 1 0 0 1	
3.165E-06	5.450E-04	50	K148	1 1 0 0 2	
3.949E-06	6.800E-04	60	K148	1 1 0 0 2	
4.652E-06	8.010E-04	70	K148	1 1 0 0 2	
5.459E-06	9.400E-04	80	K148	1 1 0 0 2	
6.261E-06	1.078E-03	90	K148	1 1 0 0 2	

2372. $C_{11}H_8O_2$
Menadione
2-Methyl-1,4-naphthoquinone
Vitamin K3
Kativ-G
Panosine
Menaphthone
RN: 58-27-5 **MP** (°C)**:** 106
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.291E-04	1.600E-01	25	P096	0 0 0 0 0	
6.969E-04	1.200E-01	30	K090	1 2 2 2 0	EFG
8.700E-04	1.498E-01	30	O321	0 0 0 0 0	
8.710E-04	1.500E-01	30	O321	0 0 0 0 0	
9.291E-04	1.600E-01	30.00	E033	1 0 2 1 0	EFG
8.888E-04	1.530E-01	33	D404	2 1 2 2 2	
8.768E-04	1.510E-01	33	D404	2 1 2 2 2	
1.161E-03	2.000E-01	37.00	E033	1 0 2 1 0	EFG

2373. $C_{11}H_8O_3$
8-Hydroxypsoralon
RN: **MP** (°C)**:**
MW: 188.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	1.148E-01	25	A355	0 0 0 0 0	

2374. $C_{11}H_8O_3$
2-Methoxy-1,4-naphthoquinone
1,4-Naphthalenedione, 2-methoxy-
2-Methoxy-1,4-naphthoquinone
RN: 2348-82-5 **MP** (°C)**:**
MW: 188.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-04	3.123E-02	ns	R427	0 0 0 0 0	

2375. $C_{11}H_9ClO_2S$
Tianafac
RN: 51527-19-6 **MP** (°C)**:**
MW: 240.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.444E-04	3.476E-02	25	C314	0 0 0 0 0	
1.442E-04	3.470E-02	25	C314	0 0 0 0 0	

2376. $C_{11}H_9Cl_2NO_2$
Barban
4-Chloro-2-butynyl-*N*-(3-chlorophenyl)carbamate
4-Chloro-2-butynyl-*m*-chlorocarbanilate
RN: 101-27-9 **MP** (°C)**:** 75
MW: 258.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.262E-05	1.100E-02	25	B200	1 0 0 0 2	
4.262E-05	1.100E-02	25	M161	1 0 0 0 1	
3.874E-05	1.000E-02	ns	H042	0 0 0 0 1	
4.262E-04	1.100E-01	ns	M061	0 0 0 0 2	

2377. $C_{11}H_9Cl_4NO_4$
OCS-21693
TMMT
Methyl-2,3,5,6-tetrachloro-*N*-methoxy-*N*-methylterephthalamate
RN: 14419-01-3 **MP** (°C)**:** 96
MW: 361.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	5.000E-03	25	B200	1 0 0 0 0	

2378. $C_{11}H_9I_3N_2O_4$
3,5-Diacetylamino-2,4,6-triiodobenzoic acid
Iothalamic acid
Diatrazoic acid
RN: 117-96-4 **MP** (°C)**:**
MW: 613.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.144E-01	5.000E+02	25	L100	1 0 0 0 2	
9.773E-01	6.000E+02	50	L100	1 0 0 0 2	
1.189E+00	7.297E+02	90	L100	1 0 0 0 2	
2.557E-03	1.570E+00	ns	H055	0 0 0 0 0	

2379. $C_{11}H_{10}$
2-Methylnaphthalene
2-Methyl naphthalene
β-Methyl naphthalenes
RN: 91-57-6 **MP** (°C)**:** 35
MW: 142.20 **BP** (°C)**:** 241.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	2.460E-02	25	E004	2 1 2 2 2	
1.828E-04	2.600E-02	25	L332	1 1 1 1 0	
1.786E-04	2.540E-02	25	M064	1 1 2 2 2	
1.800E-04	2.560E-02	25	M342	1 0 1 1 1	
1.758E-04	2.500E-02	25	O320	0 0 0 0 0	
1.786E-04	2.540E-02	ns	H123	0 0 0 0 0	
8.000E-05	1.138E-02	ns	L060	0 0 0 0 0	
1.786E-04	2.540E-02	ns	M344	0 0 0 0 2	

2380. $C_{11}H_{10}$
1-Methylnaphthalene
1-Methyl naphthalene
1-Methyl-napthalene
α-Methyl naphthalenes
α-Methylnaphthalene
RN: 90-12-0 **MP** (°C)**:** –22
MW: 142.20 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E-04	2.473E-02	4	D351	1 2 1 1 2	
1.600E-04	2.275E-02	10	S076	2 2 2 2 1	
2.000E-04	2.844E-02	14	S076	2 2 2 2 1	
1.195E-04	1.700E-02	20	A050	1 0 1 1 1	
2.145E-04	3.050E-02	20	B318	0 0 0 0 0	EFG
2.124E-04	3.020E-02	20	B356	0 0 0 0 0	
2.000E-04	2.844E-02	20	S076	2 2 2 2 1	
2.100E-04	2.986E-02	21	A057	2 1 2 2 1	

(*continued*)

2380. $C_{11}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-04	3.539E-02	25	D351	1 2 1 1 2	
1.814E-04	2.580E-02	25	E004	2 1 2 2 2	
1.899E-04	2.700E-02	25	L332	1 1 1 1 0	
2.004E-04	2.850E-02	25	M064	1 1 2 2 2	
2.000E-04	2.844E-02	25	M342	1 0 1 1 2	
2.100E-04	2.986E-02	25	S076	2 2 2 2 1	
2.440E-04	3.470E-02	28	B348	2 2 2 2 2	
2.955E-04	4.203E-02	40	D351	1 2 1 1 2	
2.004E-04	2.850E-02	ns	H123	0 0 0 0 0	
1.600E-04	2.275E-02	ns	L060	0 0 0 0 1	
2.004E-04	2.850E-02	ns	M344	0 0 0 0 2	

2381. $C_{11}H_{10}BrN_3O_2S$
5-Sulfanilamido-2-bromopyridine
Benzenesulfonamide, 4-amino-*N*-(2-bromo-5-pyridinyl)-
RN: 17103-43-4 **MP** (°C)**:**
MW: 328.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-04	1.220E-01	37	R058	1 2 1 1 2	

2382. $C_{11}H_{10}BrN_3O_2S$
2-Sulfanilamido-5-bromopyridine
Benzenesulfonamide, 4-amino-*N*-(5-bromo-2-pyridinyl)-
RN: 16805-99-5 **MP** (°C)**:**
MW: 328.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-04	3.800E-02	37	R058	1 2 1 1 1	

2383. $C_{11}H_{10}ClNO_2$
Chlorbupham
1-Methylpropyn-2-yl *N*-(*m*-chlorophenyl)carbamate
Chlorbufam
Bi-PC
RN: 1967-16-4 **MP** (°C)**:** 45.5
MW: 223.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.414E-03	5.400E-01	20	B185	0 0 0 0 0	
2.414E-03	5.400E-01	20	M161	1 0 0 0 2	

2384. $C_{11}H_{10}ClN_3O_2S$
5-Sulfanilamido-2-chloropyridine
*N*1-(6-Chloro-3-pyridyl)sulfanilamide
RN: 34392-82-0 **MP** (°C)**:**
MW: 283.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.344E-04	1.800E-01	37	R058	1 2 1 1 1	

2385. $C_{11}H_{10}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid allyl ester
Allyl 2,4-dichlorophenoxyacetate
RN: 58965-05-2 **MP** (°C)**:**
MW: 261.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	3.722E-02	ns	M120	0 0 1 1 2	

2386. $C_{11}H_{10}IN_3O_2S$
2-Sulfanilamido-5-iodopyridine
Benzenesulfonamide, 4-amino-*N*-(5-iodo-2-pyridinyl)-
RN: 71119-21-6 **MP** (°C)**:**
MW: 375.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-05	1.300E-02	37	R058	1 2 1 1 1	

2387. $C_{11}H_{10}N_2O$
3-*o*-Toluoxypyridazine
Credazine
3-(2-Methylphenoxy)-pyridazine
RN: 14491-59-9 **MP** (°C)**:** 78
MW: 186.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	1.996E+00	ns	B100	0 0 0 0 0	
1.074E-02	2.000E+00	rt	M161	0 0 0 0 0	

2388. $C_{11}H_{10}N_2O$
Vasicinone
Pyrrolo[2,1-b]quinazolin-9(1H)-one, 2,3-dihydro-3-hydroxy-, (3*S*)-
(–)-Vasicinone
L-Vasicinone
RN: 486-64-6 **MP** (°C)**:** 204
MW: 186.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-03	1.597E+00	25	B194	2 2 2 2 1	

2389. $C_{11}H_{10}N_2O_3$
Phenylmethylbarbituric acid
Barbituric acid, 5-methyl-5-phenyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-phenyl
2,4,6-Trioxo-5-methyl-5-phenylhexahydropyrimidine
Heptobarbital
RN: 76-94-8 **MP** (°C)**:** 226
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-03	7.594E-01	20	J030	1 2 2 2 1	
4.170E-03	9.100E-01	25	P350	0 0 0 0 0	intrinsic
6.133E-03	1.338E+00	37	J030	1 2 2 2 2	

2390. $C_{11}H_{10}N_2S$
1-Naphthylthiourea
ANTU
RN: 86-88-4 **MP** (°C)**:** 198
MW: 202.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.966E-03	6.000E-01	rt	M161	0 0 0 0 2	

2391. $C_{11}H_{10}N_4O_4S$
2-Sulfanilamido-5-nitropyridine
Benzenesulfonamide, 4-amino-*N*-(5-nitro-2-pyridinyl)-
RN: 39588-36-8 **MP** (°C)**:**
MW: 294.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-04	3.700E-02	37	R058	1 2 1 1 1	

2392. $C_{11}H_{11}ClO_3$
Alclofenac
(4-Allyloxy-3-chlorophenyl)acetic acid
(3-Chloro-4-allyloxyphenyl)acetic acid
RN: 22131-79-9 **MP** (°C)**:**
MW: 226.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.850E-05	1.099E-02	5	F306	1 0 1 2 2	intrinsic
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
6.200E-05	1.405E-02	25	F306	1 0 1 2 2	intrinsic
8.000E-05	1.813E-02	37	F306	1 0 1 2 2	intrinsic

2393. $C_{11}H_{11}N$
2,4-Dimethylquinoline
Quinoline, 2,4-dimethyl-
RN: 1198-37-4 **MP** (°C)**:** 264
MW: 157.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	K119	1 0 0 0 2	

2394. $C_{11}H_{11}N$
2,7-Dimethylquinoline
Quinoline, 2,7-dimethyl-
RN: 93-37-8 **MP** (°C)**:** 58
MW: 157.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	P051	2 1 1 2 2	
1.142E-02	1.795E+00	25.00	P007	2 1 2 2 2	

2395. $C_{11}H_{11}NO$
Aziridine, 1-(1-oxo-3-phenyl-2-propenyl)-
N-Cyclopropylcinnamamide
RN: 53162-40-6 **MP** (°C)**:**
MW: 173.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.150E-03	5.456E-01	ns	H350	0 0 0 0 0	

2396. $C_{11}H_{11}NO_2$

Phensuximide
Milontin
N-Methyl-2-phenyl-succinimide
RN: 86-34-0 **MP** (°C)**:** 71–73
MW: 189.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-02	4.200E+00	25	P061	0 0 0 0 0	

2397. $C_{11}H_{11}NO_2S$

Butyric acid, *p*-isothiocyanatophenyl ester
RN: 96933-13-0 **MP** (°C)**:**
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.814E-02	25	K032	2 2 0 1 1	

2398. $C_{11}H_{11}NO_4$

Acetamide, *N*-acetyl-2-(benzoyloxy)-
RN: 68659-48-3 **MP** (°C)**:** 104.5
MW: 221.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.978E-03	8.800E-01	22	N317	1 1 2 1 2	

2399. $C_{11}H_{11}NO_4S$

4-Thiazolidinecarboxylic acid, 2-(4-carboxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(4-carboxyphenyl)-
RN: 118845-10-6 **MP** (°C)**:**
MW: 253.28 **BP** (°C)**:** 551.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.520E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2400. $C_{11}H_{11}NO_5$
Benzoxydiglycine
RN: **MP** (°C)**:**
MW: 237.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E-02	3.300E+00	25.1	N026	0 0 0 0 0	

2401. $C_{11}H_{11}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-amino-2-oxoethyl ester
(*O*-Acetylsalicyloyloxy)acetamide
RN: 50785-22-3 **MP** (°C)**:** 128.5
MW: 237.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-02	3.840E+00	21	N335	0 0 0 0 0	

2402. $C_{11}H_{11}N_3OS$
Seedvax
2-Amino-4-methyl-5-carboxanilidothiazole
RN: 21452-14-2 **MP** (°C)**:** 221
MW: 233.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.282E-03	9.990E-01	ns	M061	0 0 0 0 0	

2403. $C_{11}H_{11}N_3O_2S$
Sulfapyridine
2-(Aminobenzene-4′-sulfamido)-pyridine
2-[Aminobenzol-4′-sulfamid]-pyridin
Sulphapyridine
2-Sulfapyridine
N-(2-Pyridyl)sulfanilamide
RN: 144-83-2 **MP** (°C)**:** 192
MW: 249.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-04	1.700E-01	16	H114	1 0 0 0 2	
2.006E-03	5.000E-01	20	C103	1 2 0 0 2	
1.323E-03	3.299E-01	20	D041	1 0 0 0 1	
8.023E-04	2.000E-01	20	F073	1 2 2 2 2	
1.075E-03	2.680E-01	25	C102	2 0 2 2 2	
1.049E-03	2.615E-01	25	M440	0 0 0 0 0	
1.645E-03	4.100E-01	35	H114	1 0 0 0 1	

(*continued*)

2403. $C_{11}H_{11}N_3O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-03	4.860E-01	37	C102	2 0 2 2 2	
1.805E-03	4.500E-01	37	D084	1 0 1 0 1	
1.985E-03	4.948E-01	37	F072	1 0 0 0 2	
1.985E-03	4.948E-01	37	F075	1 0 2 2 2	
2.006E-03	5.000E-01	37	F300	1 0 0 0 0	
4.047E-03	1.009E+00	37	G037	2 2 2 1 0	EFG, form V
6.128E-03	1.528E+00	37	G073	2 2 2 1 0	EFG, amorphous
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form II
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form I
2.090E-03	5.210E-01	37	K095	2 0 0 0 2	intrinsic
2.447E-03	6.100E-01	37	M057	1 0 0 0 2	pH 5.5
2.607E-03	6.500E-01	37	R044	0 0 0 0 0	
6.417E-04	1.600E-01	37.50	M142	1 0 0 0 1	
2.165E-03	5.397E-01	37.50	M142	1 0 0 0 1	
2.006E-03	5.000E-01	38	K006	1 0 0 0 2	
4.412E-03	1.100E+00	40	C103	1 2 0 0 2	
4.212E-02	1.050E+01	100	C103	1 2 0 0 2	
3.972E-02	9.901E+00	100	D041	1 0 0 0 0	
1.995E-03	4.974E-01	ns	R427	0 0 0 0 0	
1.484E-03	3.699E-01	rt	N015	0 0 2 2 2	

2404. $C_{11}H_{11}N_3O_3S_2$

Acetyl sulfathiazole
Sulfathiazol acetyle
*N*4-Acetylsulfathiazole
*N*4-Acetylsulphathiazole

RN: 127-76-4 **MP** (°C)**:**
MW: 297.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.363E-04	1.000E-01	37	D084	1 0 1 0 1	
2.186E-04	6.500E-02	37	F075	1 0 2 2 1	
2.354E-04	7.000E-02	37	L091	1 0 0 0 0	pH 5.5
1.951E-04	5.800E-02	37	M057	1 0 0 0 1	pH 5.5
2.018E-04	6.000E-02	37.50	M142	1 0 0 0 0	
2.388E-04	7.100E-02	38	K006	1 0 0 0 1	

2405. $C_{11}H_{11}N_3O_3S$

5-Sulfanilamido-2-hydroxypyridine

RN: 71119-20-5 **MP** (°C)**:**
MW: 265.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.725E-03	2.580E+00	37	R058	1 2 1 1 1	

2406. $C_{11}H_{11}N_5$
Phenazopyridine
3-(Phenylazo)-2,6-pyridinediamine
RN: 94-78-0 **MP** (°C)**:** 235
MW: 213.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.240E+00	9.042E+02	25	B443	0 0 0 0 0	
1.738E-04	3.706E-02	ns	R427	0 0 0 0 0	

2407. $C_{11}H_{12}ClNO_4$
Chloroethyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl 2-chloroethyl ester
Acetanilide, 4′-hydroxy-, 2-chloroethyl carbonate (ester)
RN: 17243-29-7 **MP** (°C)**:** 122.5–123
MW: 257.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.514E-03	3.900E-01	37	D029	0 0 0 0 0	

2408. $C_{11}H_{12}Cl_2N_2O_5$
Chloramphenicol
D-(–)-Threo-1-(*p*-nitrophenyl)-2-dichloroacetamido-1,3-propanediol
Amphicol
Leukomycin
Cloramical
Intramyctin
RN: 56-75-7 **MP** (°C)**:** 150.5
MW: 323.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.717E-03	2.494E+00	20	D041	1 0 0 0 1	
5.570E-03	1.800E+00	23	M168	2 0 0 0 0	EFG
1.200E-02	3.878E+00	25	A352	0 0 0 0 0	
7.717E-03	2.494E+00	25	I312	0 0 0 0 0	
1.156E-02	3.736E+00	25.5	J011	1 0 2 1 2	pH 4.7
1.370E-02	4.427E+00	30	K020	1 0 1 1 0	EFG
1.238E-02	4.000E+00	37	G010	1 0 1 1 0	EFG
7.737E-03	2.500E+00	ns	K444	0 0 0 0 0	

2409. $C_{11}H_{12}Cl_2O_3$
2,4-D Isopropyl ester
2,4-D-Isopropyl ester
2,4-Dichlorophenoxyacetic acid isopropyl ester
2,4-Dichlorophenoxyacetic acid *iso*-propyl ester
RN: 94-11-1 **MP** (°C)**:**
MW: 263.12 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.736E-02	ns	M120	0 0 1 1 2	
1.419E-04	3.734E-02	ns	M120	0 0 1 1 2	

2410. $C_{11}H_{12}I_3NO_2$
Iopanoic acid
β-(3-Amino-2,4,6-triiodophenyl)-α-ethylpropionic acid
Bilijodon
Cholevid
Choladine
Colepax
RN: 96-83-3 **MP** (°C)**:** 155.2
MW: 570.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	3.483E-01	37	J016	1 0 0 0 1	pH 7.4
2.627E-05	1.500E-02	ns	H055	0 0 0 0 0	

2411. $C_{11}H_{12}NO_4PS_2$
Phosmet
Phosphorodithioic scid *S*-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] *O,O*-dimethyl ester
Decemthion
Smidan
Appa
Imidan
RN: 732-11-6 **MP** (°C)**:**
MW: 317.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-05	2.440E-02	20	B300	2 1 1 1 2	
7.878E-05	2.500E-02	25	M061	1 0 0 0 1	
7.878E-05	2.500E-02	25	M161	1 0 0 0 1	
7.878E-05	2.500E-02	ns	F071	0 1 2 1 1	
7.943E-05	2.521E-02	ns	R427	0 0 0 0 0	

2412. $C_{11}H_{12}N_2O$

Antipyrine
Antipyrin
2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one
1,2-Dihydro-1,5-dimethyl-2-phenyl-3H-pyrazol-3-one
Phenazone

RN: 60-80-0 **MP** (°C)**:** 114
MW: 188.23 **BP** (°C)**:** 319

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E+00	2.918E+02	2.5	K075	1 0 0 0 2	
1.968E+00	3.705E+02	4.62	M109	2 1 1 1 0	EFG
1.472E-01	2.771E+01	5	L089	1 0 0 0 2	*sic*
1.613E+00	3.036E+02	6.1	K075	1 0 0 0 2	
1.777E-01	3.344E+01	10	L089	1 0 0 0 2	*sic*
2.084E+00	3.922E+02	11.74	M109	2 1 1 1 0	EFG
2.261E+00	4.256E+02	14.20	M109	2 1 1 1 0	EFG
1.771E+00	3.333E+02	20	D041	1 0 0 0 0	
2.205E-01	4.150E+01	20	L089	1 0 0 0 2	*sic*
2.472E+00	4.654E+02	20.96	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	25	L089	1 0 0 0 2	*sic*
3.294E+00	6.200E+02	25	P012	0 0 0 0 0	
3.294E+00	6.200E+02	25	P016	1 0 0 1 2	
3.559E+00	6.700E+02	25	P020	2 0 1 1 2	
2.717E+00	5.114E+02	25.35	M109	2 1 1 1 0	EFG
3.020E+00	5.685E+02	29.87	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	30	L089	1 0 0 0 2	*sic*
2.983E-01	5.616E+01	35	L089	1 0 0 0 2	*sic*
3.968E+00	7.468E+02	39.34	M109	2 1 1 1 0	EFG
3.359E-01	6.323E+01	40	L089	1 0 0 0 2	*sic*
5.637E-01	1.061E+02	50	L089	1 0 0 0 2	*sic*
1.493E+00	2.811E+02	.0	K075	1 0 0 0 2	
2.656E+00	5.000E+02	rt	D021	0 0 1 1 2	

2413. $C_{11}H_{12}N_2O_2$

DL-Tryptophan
1H-Indole-3-alanine
DL-α-Amino-3-indolepropionic acid

RN: 54-12-6 **MP** (°C)**:** 289
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	2.083E+00	20	N006	0 0 0 0 0	
1.140E-02	2.328E+00	25	N006	0 0 0 0 0	
1.221E-02	2.494E+00	30	D041	1 0 0 0 1	
1.250E-02	2.553E+00	30	N006	0 0 0 0 0	
1.200E-02	2.451E+00	30	N009	0 0 0 0 0	
1.640E-02	3.349E+00	40	N006	0 0 0 0 0	
1.570E-02	3.206E+00	40	N009	0 0 0 0 0	
2.150E-02	4.391E+00	50	N006	0 0 0 0 0	

2414. $C_{11}H_{12}N_2O_2$

Tryptophan
2-Amino-3-(lH-indol-3-yl)-propanoic acid
3-Indol-3-ylalanine
L-β-3-indolylalanine
Trp
(*S*)-(–)-Tryptophan

RN: 73-22-3 **MP** (°C)**:**
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-02	8.200E+00	0	F300	1 0 0 0 1	
6.042E-02	1.234E+01	20	B032	1 2 2 1 2	
6.395E-02	1.306E+01	22.5	P045	0 0 2 1 2	
6.551E-02	1.338E+01	25	B032	1 2 2 1 2	
5.519E-02	1.127E+01	25	D041	1 0 0 0 2	
5.337E-02	1.090E+01	25	F300	1 0 0 0 2	
6.665E-02	1.361E+01	25	G092	2 1 1 1 1	
6.665E-02	1.361E+01	25	G315	0 0 0 0 0	
5.519E-02	1.127E+01	25	H070	1 0 0 0 2	
6.267E-02	1.280E+01	25.1	N024	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N025	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N026	0 0 0 0 0	
6.665E-02	1.361E+01	25.1	N027	1 1 2 2 2	
1.787E-01	3.650E+01	27	D036	0 0 0 0 0	
5.386E-02	1.100E+01	28	L081	2 1 2 2 2	
7.056E-02	1.441E+01	29.80	B032	1 2 2 1 2	
8.100E-02	1.654E+01	30	N009	0 0 0 0 0	
9.480E-02	1.936E+01	40	N009	0 0 0 0 0	
8.226E-02	1.680E+01	50	F300	1 0 0 0 2	
1.122E-01	2.291E+01	50	N009	0 0 0 0 0	
1.200E-01	2.450E+01	70	F300	1 0 0 0 2	
1.334E-01	2.724E+01	75	D041	1 0 0 0 2	
2.448E-01	5.000E+01	100	F300	1 0 0 0 1	

2415. $C_{11}H_{12}N_2O_2$

5-Ethyl-5-phenylhydantoin
2,4-Imidazolidinedione, 5-ethyl-5-phenyl-
Nirvanol
5-Phenyl-5-ethylhydantoin
Normephenytoin

RN: 631-07-2 **MP** (°C)**:**
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.938E-03	8.044E-01	37	F183	1 0 1 1 1	intrinsic

2416. $C_{11}H_{12}N_2O_4$
Acetamide, *N*-(2-amino-2-oxoethyl)-2-(benzoyloxy)-
RN: 106231-53-2 **MP** (°C)**:** 151.5
MW: 236.23 **BP** (°C)**:** 568.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.175E-02	7.500E+00	22	B427	1 0 0 1 1	in 0.01M HCl
3.175E-02	7.500E+00	22	N317	1 1 2 1 2	

2417. $C_{11}H_{12}N_4O_2S$
2-Sulfanilamido-5-aminopyridine
Benzenesulfonamide, 4-amino-*N*-(5-amino-2-pyridinyl)-
RN: 16840-28-1 **MP** (°C)**:**
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-02	4.180E+00	37	R058	1 2 1 1 2	

2418. $C_{11}H_{12}N_4O_2S$
4-Sulfanilamido-2-methylpyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-methyl-4-pyrimidinyl)-
RN: 599-84-8 **MP** (°C)**:**
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.357E-02	6.230E+00	37	R046	1 2 1 1 2	

2419. $C_{11}H_{12}N_4O_2S$
Sulfamethylpyrimidine
Ulfamerazine
Sulfamerazine
RN: 127-79-7 **MP** (°C)**:** 234
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.967E-04	2.370E-01	20	F073	1 2 2 2 2	
7.641E-04	2.020E-01	20	L058	1 0 1 1 2	
8.012E-04	2.118E-01	25	M440	0 0 0 0 0	
1.400E-03	3.700E-01	37	L091	1 0 0 0 1	pH 5.5
1.203E-03	3.180E-01	37	R045	1 2 1 1 2	
1.381E-03	3.650E-01	37	S192	1 0 1 1 2	pH 6.0
1.551E-03	4.100E-01	38	K006	1 0 0 0 1	

2420. $C_{11}H_{12}N_4O_3S_2$
*N*4-Acetyl sulfamethizole
Acetyl sulfamethylthiazole
RN: 39719-87-4 **MP** (°C)**:**
MW: 312.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-03	4.100E-01	37	B046	1 0 2 2 1	pH 4.5

2421. $C_{11}H_{12}N_4O_3S$
Sulfamethoxypyridazine
Sulphamethoxypyridazine
4-Amino-*N*-(6-methoxy-3-pyridazinyl)-benzenesulfonamide
RN: 80-35-3 **MP** (°C)**:** 182.5
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.067E-03	5.795E-01	25	E314	0 0 0 0 0	intrinsic
2.569E-02	7.200E+00	37	B046	1 0 2 2 2	pH 4.5

2422. $C_{11}H_{12}N_4O_3S$
Sulfameter
Sulphamethoxydiazine
RN: 651-06-9 **MP** (°C)**:** 213
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.700E-01	30	M113	2 2 2 2 0	form III, EFG, 0.1N HCl
2.604E-03	7.300E-01	30	M113	2 2 2 2 0	form II, EFG, 0.1N HCl
1.891E-03	5.300E-01	30	M113	2 2 2 2 0	form I, EFG, 0.1N HCl
2.462E-03	6.900E-01	30	M113	2 2 2 2 0	EFG, 0.1N HCl, amorphous
3.211E-04	9.000E-02	37.5	C081	1 0 1 0 0	EFG, form III
6.243E-04	1.750E-01	37.5	C081	1 0 1 0 0	EFG, form II
4.281E-04	1.200E-01	37.5	C081	1 0 1 0 0	EFG, form I

2423. $C_{11}H_{12}N_4O_3S$
5-Sulfanilamido-2-methoxypyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-methoxy-5-pyrimidinyl)-
RN: 71119-37-4 **MP** (°C)**:**
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.282E-04	9.200E-02	37	R046	1 2 1 1 1	

2424. $C_{11}H_{12}N_4O_3S$
2-Sulfanilamido-4-methoxypyrimidine
Benzenesulfonamide, 4-amino-*N*-(4-methoxy-2-pyrimidinyl)-
RN: 3213-22-7 **MP** (°C)**:**
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.493E-04	1.820E-01	37	R046	1 2 1 1 2	

2425. $C_{11}H_{12}N_4O_5$
2,5-Diacetoxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 2,5-bis[(acetyloxy)methyl]-2,5-dihydro-
RN: 98827-24-8 **MP** (°C)**:** 153–154
MW: 280.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-02	2.900E+00	22	B322	0 0 0 0 0	

2426. $C_{11}H_{12}N_6O_2S$
6-Sulfapurine
RN: **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.447E-05	1.300E-02	20	F073	1 2 2 2 1	

2427. $C_{11}H_{12}O_2$
Cinnamyl acetate
3-Phenylallyl acetate
3-Phenyl-2-propenyl acetate
1-Acetoxy-3-phenyl-2-propene
3-Phenyl-2-propen-1-ol acetate
NSC 46109
RN: 103-54-8 **MP** (°C)**:**
MW: 176.22 **BP** (°C)**:** 170 (°50 torr)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.762E-01	25	D407	1 0 2 2 2	
1.000E-03	1.762E-01	ns	S460	0 0 0 0 0	

2428. $C_{11}H_{12}O_2$
Ethyl cinnamate
Ethyl (E)-cinnamate
Ethyl 3-phenyl propenoate
Ethyl phenylacrylate
RN: 103-36-6 **MP** (°C)**:** 6
MW: 176.22 **BP** (°C)**:** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-03	1.780E-01	25	A002	1 2 1 1 2	

2429. $C_{11}H_{12}O_4$
3,5-Dimethoxycinnamic acid
Predominantly *trans* isomer
RN: 16909-11-8 **MP** (°C)**:** 174.5
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-04	3.144E-02	25	R070	0 0 0 0 0	

2430. $C_{11}H_{12}O_4$
Ethyl acetylsalicylate
Acetyl salicylic acid, ethyl ester
RN: 529-68-0 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.594E-02	3.320E+00	37	G430	0 0 0 0 0	pH 4.5

2431. $C_{11}H_{12}O_4$
Propionyl-*r*-mandelic acid
RN: **MP** (°C)**:** 126
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-02	2.892E+00	0	A043	1 2 1 1 1	
1.389E-02	2.892E+00	0	L035	1 2 2 1 1	
1.675E-02	3.488E+00	10	A043	1 2 1 1 1	
1.675E-02	3.488E+00	10	L035	1 2 2 1 1	
1.770E-02	3.686E+00	15	A043	1 2 1 1 1	
1.770E-02	3.686E+00	15	L035	1 2 2 1 1	
1.818E-02	3.786E+00	20	A043	1 2 1 1 1	
1.818E-02	3.786E+00	20	L035	1 2 2 1 1	
2.484E-02	5.173E+00	25	A043	1 2 1 1 1	

(*continued*)

2431. $C_{11}H_{12}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-02	5.173E+00	25	L035	1 2 2 1 1	
2.817E-02	5.865E+00	30	A043	1 2 1 1 1	
2.817E-02	5.865E+00	30	L035	1 2 2 1 1	
3.528E-02	7.346E+00	35	A043	1 2 1 1 1	
3.528E-02	7.346E+00	35	L035	1 2 2 1 1	
5.789E-02	1.205E+01	40	A043	1 2 1 1 2	
5.789E-02	1.205E+01	40	L035	1 2 2 1 2	
8.724E-02	1.816E+01	45	A043	1 2 1 1 2	
8.724E-02	1.816E+01	45	L035	1 2 2 1 2	
1.606E-01	3.344E+01	50	A043	1 2 1 1 2	
1.606E-01	3.344E+01	50	L035	1 2 2 1 2	

2432. $C_{11}H_{12}O_4S$

Benzoic acid, 2-(acetyloxy)-, (methylthio)methyl ester

RN: 76432-30-9 **MP** (°C)**:**

MW: 240.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.289E-03	5.500E-01	21	N335	0 0 0 0 0	

2433. $C_{11}H_{12}O_5S$

2-(Acetoxy)-benzoic acid, (methylsulfinyl)methyl ester

RN: 76432-33-2 **MP** (°C)**:** 80.5

MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.651E-02	4.230E+00	21	N335	0 0 0 0 0	

2434. $C_{11}H_{12}O_6S$

2-(Acetoxy)-benzoic acid, (methylsulfonyl)methyl ester

RN: 76432-35-4 **MP** (°C)**:** 150

MW: 272.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-04	1.100E-01	21	N335	0 0 0 0 0	

2435. $C_{11}H_{13}ClO_3$
Bexone
4-(2-Methyl-4-chlorophenoxy)butyric acid
4-(MCPB)
MCPB
RN: 94-81-5 **MP** (°C)**:**
MW: 228.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.099E-04	4.800E-02	25	B164	1 0 1 1 1	
1.924E-04	4.400E-02	ns	L024	0 0 0 0 1	
1.924E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.924E-04	4.400E-02	rt	M161	0 0 0 0 1	

2436. $C_{11}H_{13}FN_2O_4$
1-Cyclohexyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, cyclohexyl ester
RN: 109232-74-8 **MP** (°C)**:**
MW: 256.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-03	9.200E-01	22	B332	1 1 0 0 1	pH 4.0

2437. $C_{11}H_{13}F_3N_2O_3S$
Mefluidide
N-(2,4-Dimethyl-5-(((trifluoromethyl)sulfonyl)amino)phenyl)acetamide
Vistar
Embark
MBR 12325
Methafluoridamid
RN: 53780-34-0 **MP** (°C)**:** 184
MW: 310.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.801E-04	1.800E-01	23	M161	1 0 0 0 2	

2438. $C_{11}H_{13}F_3N_4O_4$
Dinitramine
1,3-Benzenediamine, *N*1,*N*1-diethyl-2,6-dinitro-4-(trifluoromethyl)-
*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-*m*-phenylenediamine
*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-phenylenediamine
USB 3584
RN: 29091-05-2 **MP** (°C)**:** 98.5
MW: 322.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.414E-06	1.100E-03	25	M161	1 0 0 0 1	

2439. $C_{11}H_{13}NO$
N,N-Dimethylcinnamide
Cinnamic acid dimethylamide
N,N-Dimethyl-3-phenyl-2-propenamide
RN: 13156-74-6 **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-02	2.926E+00	ns	H350	0 0 0 0 0	

2440. $C_{11}H_{13}NO$
N-Ethylcinnamamide
N-Ethyl-3-phenyl-2-propenamide
RN: 23784-45-4 **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.390E-03	1.120E+00	ns	H350	0 0 0 0 0	

2441. $C_{11}H_{13}NO_2S$
2-*p*-Tolyl-4-thiazolidinecarboxylic acid
4-Thiazolidinecarboxylic acid, 2-(4-methylphenyl)-
RN: 67189-37-1 **MP** (°C)**:**
MW: 223.30 **BP** (°C)**:** 444.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.019E-01	21	B414	1 0 0 1 1	very fast and extent decomposition, uncertain value

2442. $C_{11}H_{13}NO_3$
Acetaminophen propionate
Propionic acid, *p*-acetamidophenyl ester
RN: 54942-42-6 **MP** (°C)**:** 130
MW: 207.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-03	3.200E-01	25	B010	1 1 1 1 0	

2443. $C_{11}H_{13}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-ethyl-
2-(Benzoyloxy)-*N*-ethylacetamide
RN: 64649-57-6 **MP** (°C)**:** 106
MW: 207.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.791E-03	1.200E+00	22	B427	1 0 0 1 1	in 0.01M HCl
5.791E-03	1.200E+00	22	N317	1 1 2 1 2	

2444. $C_{11}H_{13}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-dimethyl-
2-(Benzoyloxy)-*N,N*-dimethylacetamide
RN: 106231-54-3 **MP** (°C)**:** 81.5
MW: 207.23 **BP** (°C)**:** 351.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.246E-02	8.800E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.246E-02	8.800E+00	22	N317	1 1 2 1 2	

2445. $C_{11}H_{13}NO_3S$
4-Thiazolidinecarboxylic acid, 2-(4-methoxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(4-methoxyphenyl)-
RN: 65884-40-4 **MP** (°C)**:** 165–166
MW: 239.30 **BP** (°C)**:** 466.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.572E-02	21	B414	1 0 0 1 1	fast decomposition

2446. $C_{11}H_{13}NO_4$
Bendiocarb
2,2-Dimethyl-1,3-benzodioxol-4-ol methylcarbamate
Fuam
Multimet
Garvox
RN: 22781-23-3 **MP** (°C)**:** 129.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.792E-04	4.000E-02	25	M161	1 0 0 0 1	
1.792E-04	4.000E-02	25	W310	1 0 0 0 0	

2447. $C_{11}H_{13}NO_4$
N,N-Dimethyl glycolamide salicylate
2-Hydroxybenzoic acid, 2-(dimethylamino)-2-oxoethyl ester
RN: 114665-08-6 **MP** (°C)**:** 68
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-02	4.400E+00	21	B331	1 2 2 1 0	pH 7.4
1.971E-02	4.400E+00	21	B331	0 0 0 0 0	

2448. $C_{11}H_{13}NO_4$
Ethyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl ethyl ester
Acetanilide, 4′-hydroxy-, ethyl carbonate (ester)
RN: 17243-26-4 **MP** (°C)**:** 121–122
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.928E-03	1.100E+00	37	D029	0 0 0 0 0	

2449. $C_{11}H_{13}NO_4$
Dioxacarb
2-(1,3-Dioxolan-2-yl)phenyl methylcarbamate
2-(1,3-Dioxolan-2-yl)-phenyl *N*-methylcarbamate
Elocron
Famid
RN: 6988-21-2 **MP** (°C)**:** 114.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-02	6.000E+00	20	M161	1 0 0 0 0	

2450. $C_{11}H_{13}NO_4S$
4-Thiazolidinecarboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-
RN: 72678-93-4 **MP** (°C)**:**
MW: 255.29 **BP** (°C)**:** 435.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.532E+00	2.1	B414	1 0 0 1 1	fast decomposition

2451. $C_{11}H_{13}N_3O$

Ampyrone
4-Aminoantipyrine
Aminophenazone

RN: 83-07-8 **MP** (°C)**:** 109
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.053E-01	1.840E+02	5.39	M109	2 1 1 1 0	EFG
1.088E+00	2.211E+02	10.93	M109	2 1 1 1 0	EFG
1.252E+00	2.544E+02	14.20	M109	2 1 1 1 0	EFG
1.527E+00	3.103E+02	20.96	M109	2 1 1 1 0	EFG
2.076E+00	4.218E+02	25.35	M109	2 1 1 1 0	EFG
2.384E+00	4.845E+02	29.87	M109	2 1 1 1 0	EFG
2.400E-01	4.878E+01	30	I010	2 1 2 2 1	EFG, *sic*
2.862E+00	5.816E+02	39.34	M109	2 1 1 1 0	EFG

2452. $C_{11}H_{13}N_3O_3S$

Sulfamoxole
Sulfuno
N-(4,5-Dimethyloxazol-2-yl)sulfanilamide

RN: 729-99-7 **MP** (°C)**:** 193
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-03	9.610E-01	20	K028	2 1 2 1 2	pH 6.0, form I
3.430E-03	9.170E-01	20	K028	2 1 2 1 2	pH 3.8, form I
3.277E-03	8.760E-01	20	K028	2 1 2 1 2	pH 6.0, form II
3.165E-03	8.460E-01	20	K028	2 1 2 1 2	pH 3.8, form II
6.274E-03	1.677E+00	20	K028	2 1 2 1 2	pH 7.3, form I
5.447E-03	1.456E+00	20	K028	2 1 2 1 2	pH 7.3, form II
3.427E-03	9.162E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 205-211 C
3.162E-03	8.453E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 188-195 C

2453. $C_{11}H_{13}N_3O_3S$

Sulfisoxazole
4-Amino-*N*-(3,4-dimethyl-5-isoxazolyl)benzenesulfonamide
3,4-Dimethyl-5-sulfanilamidoisoxazole
Gantrisin
Urogan
Urisoxin

RN: 127-69-5 **MP** (°C)**:** 194
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-03	3.300E-01	37	B046	1 0 2 2 1	pH 4.5
3.142E-04	8.400E-02	37	K022	1 0 1 1 0	intrinsic
1.092E-03	2.920E-01	37	K091	1 0 0 0 2	

2454. $C_{11}H_{13}N_3O_3S$

*N*1-Methyl-*N*1-(5-methyl-3-isoxazolyl)sulfanilamide
*N*1-Methylsulfamethoxazole
RN: 51543-31-8 **MP** (°C)**:**
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-04	1.679E-01	37	K095	2 0 0 0 2	intrinsic

2455. $C_{11}H_{13}N_5O_2$

Carbovir
9-[4α-(Hydroxymethyl)-cyclopent-2-ene-1α-yl]guanine
RN: 118353-05-2 **MP** (°C)**:**
MW: 247.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.015E-03	1.240E+00	25	A338	0 0 0 0 0	

2456. $C_{11}H_{13}N_5O_5$

Arabinosyladenine 5′-formate
Arabinosyladenine 5′-*O*-formate ester
NSC 171240
RN: 55648-40-3 **MP** (°C)**:** 168–170
MW: 295.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-01	3.400E+01	ns	R030	0 0 0 0 0	

2457. $C_{11}H_{14}ClNO$

Propachlor
2-Chloro-*N*-isopropylacetanilide
N-Isopropyl-2-chloroacetanilide
N-Isopropyl-α-chloroacetanilide
RN: 1918-16-7 **MP** (°C)**:** 67
MW: 211.69 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-03	7.000E-01	20	B200	1 0 0 0 2	
3.307E-03	7.000E-01	20	M161	1 0 0 0 2	
3.304E-03	6.995E-01	ns	J008	0 0 0 0 0	
3.304E-03	6.995E-01	ns	M061	0 0 0 0 0	
2.362E-03	5.000E-01	ns	M110	0 0 0 0 0	EFG

2458. $C_{11}H_{14}N_2O$
Cytisine
Cytisin
RN: 485-35-8 **MP** (°C)**:** 155
MW: 190.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.308E+00	4.390E+02	16	F300	1 0 0 0 2	

2459. $C_{11}H_{14}N_2O_3S$
Sulfadicramide
2-Butenamide, *N*-[(4-aminophenyl)sulfonyl]-3-methyl-
N-Sulfanilyl-β,β-dimethylacrylamide
Sulfirgamid
Irgamide
Sulfirgamide

RN: 115-68-4 **MP** (°C)**:** 184.5
MW: 254.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-03	2.610E-01	20	F073	1 2 2 2 2	

2460. $C_{11}H_{14}N_4O_2S_2$
4-Amino-*N*-(5-isopropyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
*N*1-(5-Isopropyl-1,3,4-thiadiazol-2-yl)sulfanilamide
Sulfaisopropylthiadiazole
Glyprothiazole
PASIT
RP 2254
RN: 80-34-2 **MP** (°C)**:**
MW: 298.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.330E-04	2.187E-01	37	A046	2 0 1 1 2	

2461. $C_{11}H_{14}N_4O_2S_2$
4-Amino-*N*-(5-propyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
*N*1-(5-Propyl-1,3,4-thiadiazol-2-yl)sulfanilamide
RN: 71119-32-9 **MP** (°C)**:**
MW: 298.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.980E-04	2.680E-01	37	A046	2 0 1 1 2	

2462. $C_{11}H_{14}N_4O_3$
2-Pivaloyloxymethyl allopurinol
Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-2-yl)methyl ester
RN: 98827-15-7 **MP** (°C)**:** 180–181
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.793E-03	1.700E+00	22	B322	0 0 0 0 0	

2463. $C_{11}H_{14}N_4O_3$
1-Pivaloyloxymethyl allopurinol
Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-18-0 **MP** (°C)**:** 185–187
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.078E-03	5.200E-01	22	B322	0 0 0 0 0	

2464. $C_{11}H_{14}N_4O_5$
6-Methoxypurine arabinoside
9H-Purine, 9-β-D-arabinofuranosyl-6-methoxy-
RN: 91969-06-1 **MP** (°C)**:**
MW: 282.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.980E-02	1.406E+01	37	C348	0 0 0 0 0	pH 7.00

2465. $C_{11}H_{14}O$
o-2-Pentenylphenol
Phenol, 2-(2-pentenyl)-
RN: 62536-86-1 **MP** (°C)**:**
MW: 162.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.054E-03	3.332E-01	25	L021	1 0 0 0 0	

2466. $C_{11}H_{14}O_2$
δ-Phenylvaleric acid
Benzenepentanoic acid
5-Phenylvaleric acid
RN: 2270-20-4 **MP** (°C)**:** 59
MW: 178.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.969E-03	1.777E+00	30	D033	2 2 1 2 2	
1.159E-02	2.066E+00	40	D033	2 2 1 2 2	

2467. $C_{11}H_{14}O_2$
4-Butylbenzoic acid
RN: 20651-71-2 **MP** (°C)**:** 100
MW: 178.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-04	1.482E-01	ns	R427	0 0 0 0 0	

2468. $C_{11}H_{14}O_2$
Ethyl hydrocinnamate
Ethyl 3-phenylpropionate
Benzenepropanoic acid, ethyl ester
RN: 2021-28-5 **MP** (°C)**:**
MW: 178.23 **BP** (°C)**:** 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.234E-03	2.200E-01	25	A002	1 2 1 1 1	

2469. $C_{11}H_{14}O_3$
n-Butyl salicylate
2-Hydroxy-benzoic acid, butyl ester
Salicylic acid *n*-butyl ester
Butyl salicylate
Benzoic acid, 2-hydroxy-, butyl ester
RN: 2052-14-4 **MP** (°C)**:**
MW: 194.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	2.800E+00	37	D009	1 2 1 1 1	0.1N HCl

2470. $C_{11}H_{14}O_3$
2-Hydroxy-3-isopropyl-6-methylbenzoic acid
o-Thymotinic acid
RN: 548-51-6 **MP** (°C)**:**
MW: 194.23 **BP** (°C)**:** 316.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.57E-03	>5.00E-01	ns	B404	0 2 1 1 0	

2471. $C_{11}H_{14}O_3$
Butylparaben
Bu-paraben
Butyl 4-hydroxybenzoate
RN: 94-26-8 **MP** (°C)**:** 68.5
MW: 194.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.040E-04	1.367E-01	15	B355	0 0 0 0 0	
8.350E-04	1.622E-01	20	B355	0 0 0 0 0	
1.065E-03	2.069E-01	20	C006	1 2 1 1 2	
1.277E-03	2.481E-01	25	A059	1 0 1 1 1	
1.050E-03	2.039E-01	25	B355	0 0 0 0 0	
8.751E-04	1.700E-01	25	D081	1 2 2 1 2	
1.130E-03	2.195E-01	25	D339	0 0 0 0 0	
5.623E-04	1.092E-01	25	F322	2 0 1 1 0	EFG
1.030E-03	2.000E-01	25	O027	1 0 1 0 0	
7.465E-04	1.450E-01	25	P013	0 0 0 0 0	
1.200E-03	2.331E-01	27	B129	2 2 2 2 1	
1.200E-03	2.331E-01	27	G078	2 1 0 1 0	EFG
1.777E-03	3.452E-01	30	A059	1 0 1 1 1	
2.221E-03	4.314E-01	35	A059	1 0 1 1 1	
2.064E-03	4.009E-01	39.3	G302	2 2 2 2 0	EFG
2.610E-03	5.069E-01	40	A059	1 0 1 1 1	
7.155E-04	1.390E-01	ns	B404	0 2 1 1 0	
1.100E-03	2.137E-01	ns	G067	2 0 1 1 1	
9.989E-04	1.940E-01	rt	I404	0 0 0 0 0	Intrinsic, Average

2472. $C_{11}H_{14}O_3$
4-Methoxyphenylbutyric acid
RN: 4521-28-2 **MP** (°C)**:** 57
MW: 194.23 **BP** (°C)**:** 335

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.122E+00	9.949E+02	37	A407	2 2 2 2 2	

2473. $C_{11}H_{14}O_4$
Dimethyl carbate
Dimelone
RN: 5826-73-3 **MP** (°C)**:** 38
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-02	1.303E+01	35	M061	1 0 0 0 2	

2474. $C_{11}H_{15}BrClO_3PS$
Profenofos
O-(4-Bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl phosphorothioate
Selecron
Curacron
Polycron
RN: 41198-08-7 **MP** (°C)**:**
MW: 373.64 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.353E-05	2.000E-02	20	E048	1 2 1 1 1	
5.353E-05	2.000E-02	20	M161	1 0 0 0 1	
7.499E-05	2.802E-02	ns	S460	0 0 0 0 0	

2475. $C_{11}H_{15}BrN_2O$
Butallylonal
5-(2-Bromoallyl)-5-*sec*-butylbarbituric acid
Dial
RN: 1142-70-7 **MP** (°C)**:** 131.5
MW: 271.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.522E-03	6.840E-01	ns	T003	0 0 0 0 2	

2476. $C_{11}H_{15}FN_2O_4$
1-Hexyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, hexyl ester
RN: 66999-99-3 **MP** (°C)**:** 68
MW: 258.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.808E-03	1.500E+00	22	B332	1 1 0 0 1	pH 4.0

2477. $C_{11}H_{15}NO_2$
m-Isopropylphenyl *N*-methylcarbamate
3-Isopropylphenyl *N*-methylcarbamate
UC-10854
RN: 64-00-6 **MP** (°C)**:** 53
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.398E-04	8.500E-02	30	D089	2 2 0 0 0	
4.398E-04	8.500E-02	30	M061	1 0 0 0 1	

2478. $C_{11}H_{15}NO_2$
Butamben
4-Aminobenzoic acid butyl ester
Butyl *p*-aminobenzoate
RN: 94-25-7 **MP** (°C)**:** 58.0
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	1.990E-01	25	H008	0 0 0 0 0	
8.332E-04	1.610E-01	25	P303	0 0 0 0 0	
1.200E-03	2.319E-01	30	J018	1 2 0 1 1	0.05N NaOH
1.200E-03	2.319E-01	30	J022	1 0 2 1 1	
1.200E-03	2.319E-01	30	N045	1 2 2 2 0	EFG
1.389E-03	2.683E-01	33	P303	0 0 0 0 0	
1.720E-03	3.324E-01	37	F006	1 1 2 2 2	
1.700E-03	3.285E-01	37	J026	2 2 2 1 1	
2.221E-03	4.293E-01	40	P303	0 0 0 0 0	
6.468E-04	1.250E-01	ns	B404	0 2 1 1 0	
7.140E-04	1.380E-01	ns	M066	0 0 0 0 2	
7.140E-04	1.380E-01	rt	B016	0 0 1 1 2	pH 7.4
7.784E-04	1.504E-01	rt	I404	0 0 0 0 0	Average

2479. $C_{11}H_{15}NO_2S$
Ethiofencarb
2-((Ethylthio)methyl)phenyl methylcarbamate
Ethylmercaptomethylphenyl-*N*-methylcarbamate
Ethiophencarp
Croneton
HOX 1901
RN: 29973-13-5 **MP** (°C)**:** <25
MW: 225.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.078E-03	1.820E+00	20	M161	1 0 0 0 2	

2480. $C_{11}H_{15}NO_3$
α,3-*o*-Isopropylidene pyriridoxine
RN: **MP** (°C)**:**
MW: 209.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-02	2.503E+00	37	M067	2 0 1 1 2	

2481. $C_{11}H_{15}NO_3$
Propoxur
o-Isopropoxyphenyl methylcarbamate
Baygon
Blattanex
Blattosep
Suncide
RN: 114-26-1 **MP** (°C)**:** 91
MW: 209.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.301E-03	1.737E+00	10	B324	0 0 0 0 0	
8.316E-03	1.740E+00	10	B324	0 0 0 0 0	
8.885E-03	1.859E+00	20	B300	2 2 1 1 2	
9.244E-03	1.934E+00	20	B324	0 0 0 0 0	
9.206E-03	1.926E+00	20	B324	0 0 0 0 0	
9.558E-03	2.000E+00	20	M161	1 0 0 0 0	
1.166E-02	2.440E+00	30	B324	0 0 0 0 0	
1.163E-02	2.434E+00	30	B324	0 0 0 0 0	
4.732E-02	9.901E+00	ns	M061	0 0 0 0 0	approximate
4.301E-04	9.000E-02	ns	M110	0 0 0 0 0	EFG

2482. $C_{11}H_{15}NO_4$
n-Ethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone
RN: **MP** (°C)**:**
MW: 225.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.908E-01	6.550E+01	20	K050	1 1 1 1 2	

2483. $C_{11}H_{15}N_3O_2$
Formetanate
Methylcarbamic acid, ester with *N′*-(*m*-hydroxyphenyl)-*N,N*-dimethylformamidine
RN: 22259-30-9 **MP** (°C)**:** 102.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E-03	1.000E+00	rt	M161	0 0 0 0 0	

2484. $C_{11}H_{15}N_3O_3$
Orotic acid cyclohexylamide
Orotamide, *N*-cyclohexyl-
RN: 4558-58-1 **MP** (°C)**:** 284–285
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-02	1.779E+01	–4	N018	0 0 0 0 0	
1.100E-01	2.610E+01	16	N018	0 0 0 0 0	
1.330E-01	3.156E+01	25	N018	0 0 0 0 0	

2485. $C_{11}H_{15}N_3O_5$
Triglycidylurazol
Anaxirone
RN: 77658-97-0 **MP** (°C)**:** 91
MW: 269.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.426E-04	2.000E-01	ns	D319	0 0 0 0 0	

2486. $C_{11}H_{15}O_3P$
Diethyl benzoyl phosphonate
Methylene, (diethoxyphosphinyl)phenyl-
RN: 105394-75-0 **MP** (°C)**:**
MW: 226.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<8.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

2487. $C_{11}H_{16}$
tert-Amylbenzene
t-Amylbenzene
RN: 2049-95-8 **MP** (°C)**:** –57.8
MW: 148.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.083E-05	1.050E-02	25	A002	1 2 1 1 2	

2488. $C_{11}H_{16}$
Amylbenzene
n-Pentylbenzene
Pentylbenzene
n-Amylbenzene
n-Pentylbenzene1-phenylpentane
RN: 538-68-1 **MP** (°C)**:** –75
MW: 148.25 **BP** (°C)**:** 205.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-05	3.481E-03	7	O312	2 2 0 2 2	
2.144E-05	3.178E-03	10	O312	2 2 0 2 2	
2.323E-05	3.444E-03	12.5	O312	2 2 0 2 2	
2.153E-05	3.192E-03	15	O312	2 2 0 2 2	
2.311E-05	3.426E-03	17.5	O312	2 2 0 2 2	
2.142E-05	3.176E-03	20	O312	2 2 0 2 2	
2.590E-05	3.840E-03	25	M342	1 0 1 1 2	
2.276E-05	3.374E-03	25	O312	2 2 0 2 2	
2.433E-05	3.607E-03	30	O312	2 2 0 2 2	
2.642E-05	3.917E-03	35	O312	2 2 0 2 2	
2.868E-05	4.252E-03	40	O312	2 2 0 2 2	
3.163E-05	4.689E-03	45	O312	2 2 0 2 2	
6.000E-03	8.895E-01	ns	H307	0 0 0 0 0	

2489. $C_{11}H_{16}$
Pentamethylbenzene
1,2,3,4,5-Pentamethyl benzene
RN: 700-12-9 **MP** (°C)**:** 50.8
MW: 148.25 **BP** (°C)**:** 231.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	1.552E-02	ns	D001	0 0 0 0 2	

2490. $C_{11}H_{16}ClO_2PS_3$
Carbophenothion
O,O-Diethyl *S*-(4-chlorophenylthiomethyl) dithiophosphate
Trithion
Garrathion
Nephocarp
Lethox
RN: 786-19-6 **MP** (°C)**:** <25
MW: 342.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B300	2 1 1 1 2	

(*continued*)

2490. $C_{11}H_{16}ClO_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.837E-06	6.300E-04	20	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
<1.17E-04	<4.00E-02	ns	M161	0 0 0 0 0	

2491. $C_{11}H_{16}N_2O_2$
4-Aminobenzoic acid-2-(ethyl-amino)ethyl ester
2-(Ethylamino)ethyl 4-aminobenzoate
RN: **MP** (°C)**:**
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-02	5.623E+00	ns	M066	0 0 0 0 1	

2492. $C_{11}H_{16}N_2O_2$
Aminocarb
Phenol, 4-(dimethylamino)-3-methyl, methylcarbamate (ester)
Carbamic acid, methyl-, 4-(dimethylamino)-*m*-tolyl ester
RN: 2032-59-9 **MP** (°C)**:** 93
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.187E-03	8.720E-01	10	B324	0 0 0 0 0	
4.183E-03	8.712E-01	10	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B300	2 2 1 1 2	
4.389E-03	9.142E-01	20	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B324	0 0 0 0 0	
4.393E-03	9.150E-01	20	G300	1 0 0 0 2	
6.521E-03	1.358E+00	30	B324	0 0 0 0 0	
6.540E-03	1.362E+00	30	B324	0 0 0 0 0	

2493. $C_{11}H_{16}N_2O_3$
Vinbarbital
5-Ethyl-5-(1-methyl-1-butenyl)barbituric acid
RN: 125-42-8 **MP** (°C)**:** 161
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-03	7.000E-01	25	B011	2 0 0 1 0	
3.164E-03	7.097E-01	25	B065	1 1 1 1 1	
4.870E-03	1.092E+00	25	V033	2 0 1 1 2	

(*continued*)

2493. $C_{11}H_{16}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.099E+00	25.00	T303	1 0 0 0 1	
7.000E-03	1.570E+00	35.00	T303	1 0 0 0 1	
8.000E-03	1.794E+00	45.00	T303	1 0 0 0 1	

2494. $C_{11}H_{16}N_2O_3$
5-Allyl-5-butylbarbituric acid
n-Butylallylbarbitone
n-Butylallylbarbituric acid
Allylbutylbarbituric acid
Idobutal
RN: 3146-66-5 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.723E-03	1.508E+00	20	J030	1 2 2 2 2	
8.945E-03	2.006E+00	37	J030	1 2 2 2 2	

2495. $C_{11}H_{16}N_2O_3$
Talbutal
Allyl-*sec*-butyl-barbituric acid
5-Allyl-5-*sec*-butylbarbituric acid
RN: 115-44-6 **MP** (°C)**:** 109
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.632E-03	2.160E+00	ns	T003	0 0 0 0 2	

2496. $C_{11}H_{16}N_2O_3$
Butalbital
Itobarbital
5-Allyl-5-isobutylbarbituric acid
Fioricet
Phrenilin
Medigesic
RN: 77-26-9 **MP** (°C)**:** 138
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.590E-03	1.702E+00	25	V033	2 0 1 1 2	
7.600E-03	1.704E+00	25.00	T303	1 0 0 0 1	
1.030E-02	2.310E+00	35.00	T303	1 0 0 0 2	
1.410E-02	3.162E+00	45.00	T303	1 0 0 0 2	

2497. $C_{11}H_{16}N_2O_3$
2,4-Diazaspiro[5.7]tridecane-1,3,5-trione
RN: 143288-62-4 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-03	2.337E-01	25	P350	0 0 0 0 0	intrinsic

2498. $C_{11}H_{16}N_2O_3$
Barbituric acid, 5-ethyl-5-(3-methyl-2-butenyl)
5-Ethyl-5-(3′-methylbut-2′-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)-
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)
5-Ethyl-5-(3-methylbut-2-enyl)barbiturate
RN: 21149-88-2 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.583E-03	1.252E+00	25	P350	0 0 0 0 0	intrinsic

2499. $C_{11}H_{16}N_2O_3S$
Phenbutamide
N-(Phenylsulfonyl)-*N′*-butylurea
N-Benzenesulfonyl-*N′*-*n*-butylurea
RN: 3149-00-6 **MP** (°C)**:** 131
MW: 256.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.995E-04	2.306E-01	37	A028	1 0 2 1 2	intrinsic
9.000E-04	2.307E-01	37	A046	2 0 1 1 2	

2500. $C_{11}H_{16}N_2O_4$
Methyl-2-ethyl-2-allylmalonurate
Methyl 2-ethyl-2-allylmalonurate
RN: 73632-83-4 **MP** (°C)**:** 78.5
MW: 240.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	2.883E+00	23	B152	1 2 1 1 1	pH 3.5

2501. $C_{11}H_{16}N_2O_5$
Methoxycarbonylmethyl-2,2-diethylmalonurate
Methoxycarbonylmethyl 2,2-diethylmalonurate
RN: **MP** (°C)**:** 89
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-03	2.486E+00	23	B152	1 2 1 1 1	pH 3.5

2502. $C_{11}H_{16}N_4O_2$
1-Butyl theobromine
1-Butyl-3,7-dimethylxanthine
1-*n*-Butyl-3,7-dimethylxanthine
RN: 1143-30-2 **MP** (°C)**:** 108
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.370E-02	5.600E+00	30	B042	1 2 1 1 2	

2503. $C_{11}H_{16}N_4O_4$
2,6-Piperazinedione, 4,4′-(1-methyl-1,2-ethanediyl)*bis*-
1,2-Di(4-piperazine-2,6-dione)propane
2,6-Piperazinedione, 4,4′-(1-methyl-1,2-ethanediyl)*bis*-, (±)-, polymer with 1,3-dibromopropane
Propane, 1,3-dibromo-, polymer with (±)-4,4′-(1-methyl-1,2-ethanediyl)bis[2,6-piperazinedione]
RN: 21416-67-1 **MP** (°C)**:** 192 dec
MW: 268.27 **BP** (°C)**:** 233 dec

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-02	3.000E+00	25	P326	0 0 0 0 0	
~5.59E-02	~1.50E+01	25	R017	0 0 0 0 0	enantimer (R)
~1.12E-02	~3.00E+00	25	R017	0 0 0 0 0	

2504. $C_{11}H_{16}O$
p-sec-Amylphenol
4-*sec*-Amylphenol
RN: 25735-67-5 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.408E-04	1.053E-01	25	L021	1 0 0 0 0	

2505. $C_{11}H_{16}O$
p-*n*-Amylphenol
4-*n*-Pentylphenol
RN: 14938-35-3 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.088E-04	9.999E-02	25	L022	1 0 0 0 0	

2506. $C_{11}H_{16}O$
p-*tert*-Pentylphenol
p-(α,α-Dimethylpropyl)phenol
p-(1,1-Dimethylpropyl)phenol
1-Hydroxy-4(2-methyl-2-butyl)benzene
PTAP
RN: 80-46-6 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	
1.023E-03	1.680E-01	25	M127	1 0 0 0 2	

2507. $C_{11}H_{16}O$
4-(1,1-Dimethylethyl)benzenemethanol
4-(1,1-Dimethylethyl)benzyl alcohol
4-*tert*-Butylbenzyl alcohol
4-*tert*-Butylphenylmethanol
p-*tert*-Butylbenzyl alcohol
RN: 877-65-6 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:** 250.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.051E+00	20	B407	1 0 1 2 2	

2508. $C_{11}H_{16}O$
o-*n*-Amylphenol
2-*n*-Amylphenol
RN: 87-26-3 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.365E-04	1.538E-01	25	L022	1 0 0 0 0	

2509. $C_{11}H_{16}O$
o-2-Hexenylphenol
2-2-Hexenylphenol
RN: 75121-79-8 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	

2510. $C_{11}H_{16}O$
2-Methyl-5-*t*-butylphenol
5-*tert*-Butyl-2-methylphenol
5-*tert*-Butyl-*o*-cresol
o-Cresol, 5-*tert*-butyl-
RN: 5781-02-2 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-03	4.160E-01	25	M127	1 0 0 0 2	

2511. $C_{11}H_{16}O_2$
4-*n*-Amyl resorcinol
4-*n*-Amyl-resorcin
RN: 533-24-4 **MP** (°C)**:**
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	2.000E+00	20	F300	1 0 0 0 0	

2512. $C_{11}H_{16}O_2$
3-Pentoxyphenol
m-Pentoxy phenol
Phenol, 3-pentoxy-
RN: 18979-73-2 **MP** (°C)**:**
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-03	3.839E-01	30	B315	0 0 0 0 0	

2513. $C_{11}H_{17}NO_3$
Dimetan
5,5-Dimethyldihydroresorcinyl *N,N*-dimethylcarbamate
RN: 122-15-6 **MP** (°C)**:** 45.5
MW: 211.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	2.913E+01	ns	M061	0 0 0 0 0	approximate

2514. $C_{11}H_{17}N_3O_3$
Orotic acid triethylamide
RN: **MP** (°C)**:** 200–202
MW: 239.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E+00	5.410E+02	25	N018	0 0 0 0 0	

2515. $C_{11}H_{17}N_3O_3S$
Carbutamide
4-Amino-*N*-[(butylamino)carbonyl]-benzenesulfonamide
1-Butyl-3-sulfanilyl urea
RN: 339-43-5 **MP** (°C)**:** 144.5
MW: 271.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.972E-03	5.352E-01	37	A028	1 0 2 1 2	intrinsic
1.950E-03	5.291E-01	37	A046	2 0 1 1 2	
6.634E-03	1.800E+00	37	C054	2 0 2 1 2	0.1N HCl

2516. $C_{11}H_{17}N_3O_6$
Orotic acid triethanolamide
RN: **MP** (°C)**:** 104–108
MW: 287.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E+00	3.778E+02	–4	N018	0 0 0 0 0	
1.882E+00	5.407E+02	16	N018	0 0 0 0 0	
2.187E+00	6.283E+02	25	N018	0 0 0 0 0	

2517. $C_{11}H_{17}O_3PS$
Kitazin
O,O-Diethyl *S*-benzyl thiophosphate
EBP
S-Benzyl *O,O*-di-ethyl phosphorothioate
RN: 13286-32-3 **MP** (°C)**:**
MW: 260.29 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	22	K137	1 1 2 1 0	

2518. $C_{11}H_{17}O_3PS_2$
Fensulfothion sulfide
O,O-Diethyl *O*-[*p*-(methylthio)phenyl] phosphorothioate
Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylthio)phenyl] ester
RN: 3070-15-3 **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E-05	3.700E-03	20	M318	2 2 0 0 2	

2519. $C_{11}H_{17}O_4PS_2$
Fensulfothion
O,O-Diethyl *O*-(4-(methylsulfinyl)phenyl) phosphorothioate
Dasanit
Bay 25141
Agricur
Chemagro 25141
RN: 115-90-2 **MP** (°C)**:** <25
MW: 308.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.473E-03	1.996E+00	20	B169	2 2 1 1 2	
6.473E-03	1.996E+00	20	F318	2 2 0 0 2	
4.994E-03	1.540E+00	25	M161	1 0 0 0 2	

2520. $C_{11}H_{17}O_5PS_2$
Fensulfothion sulfone
Phosphorothioic acid, *O,O*-diethyl *O*-[*p*-(methylsulfonyl)phenyl] ester
Dasanit sulfone
Dasanit sulphone
RN: 14255-72-2 **MP** (°C)**:**
MW: 324.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.242E-04	4.030E-02	10	B324	0 0 0 0 0	
1.243E-04	4.032E-02	10	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	B169	2 2 1 1 2	
2.633E-04	8.540E-02	20	B324	0 0 0 0 0	
2.633E-04	8.539E-02	20	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	M318	2 2 0 0 2	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	

2521. $C_{11}H_{18}N_2O_2S$
Thiopental
5-Ethyl-5-(1-methyl-butyl)-2-thiobarbituric acid
5-Ethyl-5-(1-methylbutyl)-2-thiobarbituric acid
Barbituric acid, 5-ethyl-5-(1-methylbutyl)-2-thio
4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(1-methylbutyl)-2-thioxo
Pentothiobarbital
RN: 76-75-5 **MP** (°C)**:** 158
MW: 242.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.063E-04	5.000E-02	25	A023	1 0 0 1 1	
3.301E-04	8.000E-02	25	B011	2 0 0 1 0	
3.333E-04	8.077E-02	25	B065	1 1 1 1 1	
8.200E-04	1.987E-01	25	G003	1 1 1 1 1	pH 4.7
2.094E-04	5.075E-02	25	P350	0 0 0 0 0	intrinsic
3.000E-04	7.270E-02	30	K108	1 2 2 0 0	
3.301E-04	7.999E-02	35	A023	1 0 0 1 1	
4.126E-04	9.999E-02	40	A023	1 0 0 1 1	

2522. $C_{11}H_{18}N_2O_3$
Amobarbital
5-Ethyl-5-isoamylbarbituric acid
Amylobarbitone
RN: 57-43-2 **MP** (°C)**:** 157
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-03	6.400E-01	20	J030	1 2 2 2 1	
3.533E-03	7.994E-01	25	A023	1 0 0 1 1	
2.475E-03	5.600E-01	25	B011	2 0 0 1 0	
2.665E-03	6.030E-01	25	B065	1 1 1 1 1	
3.900E-03	8.825E-01	25	G003	1 1 1 1 1	pH 4.7
2.170E-03	4.910E-01	25	V033	2 0 1 1 2	
2.200E-03	4.978E-01	25.00	T303	1 0 0 0 1	
3.000E-03	6.788E-01	30	G014	1 1 1 1 0	EFG
3.100E-03	7.015E-01	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
2.846E-03	6.440E-01	30	I015	1 2 2 1 2	pH 6.0, 3 forms
3.200E-03	7.241E-01	30	K108	1 2 2 0 1	
3.300E-03	7.467E-01	35.00	T303	1 0 0 0 1	
4.375E-03	9.900E-01	37	J030	1 2 2 2 1	
4.000E-03	9.051E-01	37	K121	1 2 1 2 0	0.1N HCl
5.517E-03	1.248E+00	40	A023	1 0 0 1 1	
3.820E-02	8.644E+00	40	N008	1 0 1 1 2	*sic*
4.300E-03	9.730E-01	45.00	T303	1 0 0 0 1	
2.342E-03	5.300E-01	ns	T003	0 0 0 0 2	

2523. $C_{11}H_{18}N_2O_3$
Pentobarbital
5-ethyl-5-(1-methyl-butyl)-barbituric acid
RN: 76-74-4 **MP** (°C)**:** 130
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.415E-03	9.990E-01	25	A023	1 0 0 1 1	
2.210E-03	5.000E-01	25	B011	2 0 0 1 0	
2.221E-03	5.026E-01	25	B065	1 1 1 1 1	
3.000E-03	6.788E-01	25	G003	1 1 1 1 1	pH 4.7
4.070E-03	9.210E-01	25	V033	2 0 1 1 2	
4.100E-03	9.277E-01	25.00	T303	1 0 0 0 1	
6.000E-03	1.358E+00	30	K108	1 2 2 0 1	
6.178E-03	1.398E+00	35	A023	1 0 0 1 1	
5.700E-03	1.290E+00	35.00	T303	1 0 0 0 1	
7.000E-03	1.584E+00	37	K121	1 2 1 2 0	0.1N HCl
7.060E-03	1.597E+00	40	A023	1 0 0 1 1	
7.640E-02	1.729E+01	40	N008	1 0 1 1 2	*sic*
6.900E-03	1.561E+00	45.00	T303	1 0 0 0 1	
4.365E-03	9.877E-01	ns	R427	0 0 0 0 0	

2524. $C_{11}H_{18}N_2O_3$
5-*n*-Pentyl-5-ethylbarbituric acid
5-Ethyl-5-pentylbarbituric acid
5-Ethyl-5-pentylbarbiturate
RN: 115-58-2 **MP** (°C)**:** 135.5
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.657E-03	1.506E+00	25	B065	1 2 1 1 1	
2.448E-03	5.540E-01	ns	T003	0 0 0 0 2	

2525. $C_{11}H_{18}N_2O_3$
Pilocarpic acid
1,2-Secopilocarpin-2-oic acid
RN: 28406-15-7 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-04	1.200E-01	23	B340	1 1 2 1 1	pH 9

2526. $C_{11}H_{18}N_4O_2$
Pirimicarb
2-(Dimethylamino)-5,6-dimethyl-4-pyrimidinyl dimethylcarbamate
Abol
Rapid
Fernos
Aphox
RN: 23103-98-2 **MP** (°C)**:** 90.5
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.700E+00	25	M161	1 0 0 0 1	

2527. $C_{11}H_{19}N_3O$
Dimethirimol
2-Dimethylamino-4-hyroxy-5-*n*-butyl-6-methylpyrimidine
RN: 5221-53-4 **MP** (°C)**:** 102
MW: 209.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.734E-03	1.200E+00	25	M161	1 0 0 0 1	
5.727E-03	1.199E+00	ns	M061	0 0 0 0 1	

2528. $C_{11}H_{19}N_3O$
Ethirimol
5-Butyl-2-(ethylamino)-4-hydroxy-6-methylpyrimidine
Milgo
Milcurb super
Milstem
RN: 23947-60-6 **MP** (°C)**:** 159.5
MW: 209.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.556E-04	2.000E-01	rt	M161	0 0 0 0 0	

2529. $C_{11}H_{20}$
2-Methyldecalin
Decahydro-2-methylnaphthalene
RN: 2958-76-1 **MP** (°C)**:**
MW: 152.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-07	4.060E-05	25	B069	1 0 1 1 2	

2530. $C_{11}H_{20}ClN_5$
Chlorazine
2-Chloro-4-diethylamino-6-diethylamino-*s*-triazine
2-Chloro-4,6-*bis*-(diethylamino)-*s*-triazine chlorazine
1,3,5-Triazine
1,3,5-Triazine-2,4-diamine
RN: 580-48-3 **MP** (°C)**:**
MW: 257.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-05	9.000E-03	20	J033	0 0 0 0 0	
3.879E-05	1.000E-02	21	B192	0 0 0 0 1	
3.492E-05	9.000E-03	21	G099	2 0 0 1 0	

2531. $C_{11}H_{20}N_2O_4$
Isopropyl-2,2-diethylmalonurate
Isopropyl 2,2-diethylmalonurate
RN: 73632-77-6 **MP** (°C)**:** 99.5
MW: 244.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	4.153E-01	23	B152	1 2 1 1 1	pH 3.5

2532. $C_{11}H_{20}N_3O_3PS$
Pirimiphos-methyl
Pirimiphosmethyl
RN: 29232-93-7 **MP** (°C)**:** 15
MW: 305.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.139E-05	2.180E-02	10	B324	0 0 0 0 0	
7.946E-05	2.426E-02	10	B324	0 0 0 0 0	
7.363E-05	2.248E-02	20	B300	2 1 1 1 2	
1.119E-04	3.417E-02	20	B324	0 0 0 0 0	
1.005E-04	3.070E-02	20	B324	0 0 0 0 0	
1.640E-04	5.008E-02	30	B324	0 0 0 0 0	
1.474E-04	4.500E-02	30	B324	0 0 0 0 0	
1.638E-05	5.000E-03	30	M161	1 0 0 0 0	*sic*

2533. $C_{11}H_{20}N_6$
1-(Pyrrolidinyl)-3,5-bis(dimethylamino)-*s*-triazine
1-Pyrrolidino-3,5-bis(dimethylamino)-*s*-triazine
RN: 13452-85-2 **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	3.878E-02	25	B386	0 0 0 0 0	

2534. $C_{11}H_{20}N_6O$
1-(Morpholinyl)-3,5-bis(dimethylamino)-*s*-triazine
s-Triazine, 2,4-bis(dimethylamino)-6-morpholino-
RN: 16269-02-6 **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-03	3.288E-01	25	B386	0 0 0 0 0	

2535. $C_{11}H_{20}N_6S$
1-(Thiomorpholinyl)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, *N,N,N′,N′*-tetramethyl-6-(4-thiomorpholinyl)-
RN: 41492-69-7 **MP** (°C)**:**
MW: 268.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.689E-05	1.527E-02	25	B386	0 0 0 0 0	

2536. $C_{11}H_{20}O_2$
Undecylenic acid
10-Undecylenic acid
Hendecenoic acid
RN: 112-38-9 **MP** (°C)**:** 25
MW: 184.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	7.371E-02	30	D051	2 0 0 1 2	
1.074E-04	1.980E-02	30	E005	2 1 1 2 2	
1.248E-04	2.300E-02	40	E005	2 1 1 2 1	
1.411E-04	2.600E-02	50	E005	2 1 1 2 1	
1.000E-03	1.843E-01	60	D051	2 0 0 1 2	
1.736E-04	3.200E-02	60	E005	2 1 1 2 1	

2537. $C_{11}H_{20}O_4$
Hexyl α-acetoxypropionate
Propanoic acid, 2-(acetyloxy)-, hexyl ester
RN: 96884-73-0 **MP** (°C)**:**
MW: 216.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-04	2.000E-01	25	R006	2 2 0 1 1	

2538. $C_{11}H_{20}O_4$
Undecanedioic acid
1,9-Nonanedicarboxylic acid
Nonan-dicarbonsaeure-(1,9)
RN: 1852-04-6 **MP** (°C)**:**
MW: 216.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.358E-02	5.100E+00	21	B040	1 0 1 1 1	*sic*
6.473E-04	1.400E-01	ns	F300	0 0 0 0 2	

2539. $C_{11}H_{20}O_5$
Propanoic acid, 2-[(hexthoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 232.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.305E-04	9.999E-02	25	R007	0 0 0 0 0	

2540. $C_{11}H_{21}BrO_2$
11-Bromoundecanoic acid
Bromo-11-undecanoique acide
RN: 2834-05-1 **MP** (°C)**:** 49.5
MW: 265.20 **BP** (°C)**:** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.304E-02	30	D051	2 0 0 1 2	
7.500E-04	1.989E-01	60	D051	2 0 0 1 2	

2541. $C_{11}H_{21}NOS$
Cycloate
S-Ethyl *N*-ethylthiocyclohexanecarbamate
RO-Neet
S-Ethyl *N,N*-ethylcyclohexylthiocarbamate
RN: 1134-23-2 **MP** (°C)**:** 12
MW: 215.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.947E-04	8.500E-02	22	B200	1 0 0 0 1	
3.947E-04	8.500E-02	22	F019	1 0 0 0 1	
3.947E-04	8.500E-02	22	M161	1 0 0 0 1	

2542. $C_{11}H_{21}NO_3$
Dipropylaceturethane
RN: **MP** (°C)**:**
MW: 215.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-03	3.998E-01	20	O021	1 2 0 0 0	

2543. $C_{11}H_{21}N_5O$
Ipatone
1,3,5-Triazine, 2-(diethylamino)-4-(isopropylamino)-6-methoxy
1,3,5-Triazine-2,4-diamine, *N,N*-diethyl-6-methoxy-*N′*-(1-methylethyl)
RN: 3004-70-4 **MP** (°C)**:**
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-04	1.000E-01	20	J033	0 0 0 0 0	

2544. $C_{11}H_{21}N_5OS$
Gesaran
2-Methylthio-4-isopropylamino-6-(3-methoxypropylamino)-*s*-triazine
Methoprotryne
RN: 841-06-5 **MP** (°C)**:** 69
MW: 271.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-03	3.200E-01	20	F311	1 2 2 2 1	
1.179E-03	3.200E-01	20	M161	1 0 0 0 2	
1.179E-03	3.200E-01	ns	J033	0 0 0 0 0	
3.681E-03	9.990E-01	ns	M061	0 0 0 0 0	

2545. $C_{11}H_{21}N_5S$
Dimethametryn
N-(1,2-Dimethylpropyl)-*N′*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Belclene 310
RN: 22936-75-0 **MP** (°C)**:**
MW: 255.39 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-04	5.000E-02	20	M161	1 0 0 0 1	

2546. $C_{11}H_{21}N_5S$
Dipropetryn
2-(Ethylthio)-4,6-bis(isopropylamino)-*s*-triazine
Cotofor
Sancap
Sancap 80W
RN: 4147-51-7 **MP** (°C)**:** 105
MW: 255.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.600E-02	rt	M161	0 0 0 0 1	

2547. $C_{11}H_{21}N_5S$
Ipatryne
2-Methylmercapto-4-isopropylamino-6-diethylamino-*s*-triazine
RN: **MP** (°C)**:**
MW: 255.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.363E-03	26	G001	1 0 1 1 1	

2548. $C_{11}H_{21}N_7$
1-(1-Piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, *N,N,N′,N′*-tetramethyl-6-(1-piperazinyl)-
RN: 125867-94-9 **MP** (°C)**:**
MW: 251.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-02	2.717E+00	25	B386	0 0 0 0 0	

2549. $C_{11}H_{21}O_5$
Propanoic acid, 2-[(proxycarbonyl)oxy]-, butyl ester
RN: **MP** (°C)**:**
MW: 233.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-04	9.999E-02	25	R007	0 0 0 0 0	

2550. $C_{11}H_{22}N_2O$
Cycluron
N′-Cyclooctyl-*N,N*-dimethylurea
Cyclooctyl-1,1-dimethylurea
OMU
RN: 2163-69-1 **MP** (°C)**:** 138
MW: 198.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.564E-04	1.500E-01	20	B185	0 0 0 0 0	
6.051E-03	1.200E+00	20	G036	1 0 0 0 2	
5.541E-03	1.099E+00	20	M061	1 0 0 0 1	
5.547E-03	1.100E+00	20	M161	1 0 0 0 1	
6.310E-04	1.251E-01	ns	M163	0 0 0 0 0	EFG

2551. $C_{11}H_{22}N_6$
*N*6,*N*6-Diethyl-*N*2,*N*2,*N*4,*N*4-tetramethylmelamine
1,3,5-Triazine-2,4,6-triamine, *N,N*-diethyl-*N′,N′,N″,N″*-tetramethyl-
RN: 16268-75-0 **MP** (°C)**:** 42.0
MW: 238.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-04	7.100E-02	25	C051	1 2 1 1 1	pH 7

2552. $C_{11}H_{22}O_2$

Undecanoic acid
Undecanoique acide

RN: 112-37-8 **MP** (°C)**:** 28.5
MW: 186.30 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.382E-03	6.300E-01	0	B136	1 0 2 1 1	
5.744E-04	1.070E-01	20	B136	1 0 2 1 2	
4.992E-04	9.299E-02	20.0	R001	1 1 1 1 1	
6.978E-04	1.300E-01	30	B136	1 0 2 1 2	
2.800E-04	5.216E-02	30	D051	2 0 0 1 2	
5.904E-04	1.100E-01	30.0	R001	1 1 1 1 1	
7.730E-04	1.440E-01	40	B136	1 0 2 1 2	
6.978E-04	1.300E-01	45	B136	1 0 2 1 1	
6.977E-04	1.300E-01	45.0	R001	1 1 1 1 1	
8.052E-04	1.500E-01	60	B136	1 0 2 1 1	
6.000E-04	1.118E-01	60	D051	2 0 0 1 2	
8.050E-04	1.500E-01	60.0	R001	1 1 1 1 1	
3.381E-04	6.300E-02	.0	R001	1 1 1 1 1	

2553. $C_{11}H_{22}O_2$

Methyl caprate
Capric acid methyl ester
Methyl decanoate

RN: 110-42-9 **MP** (°C)**:** –13
MW: 186.30 **BP** (°C)**:** 223

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.36E-05	<4.40E-03	20	M337	2 1 2 2 1	
2.051E-05	3.821E-03	ns	S460	0 0 0 0 0	

2554. $C_{11}H_{22}O_2$

Ethyl nonanoate
Ethyl nonylate

RN: 123-29-5 **MP** (°C)**:**
MW: 186.30 **BP** (°C)**:** 119 at 23 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-04	2.953E-02	ns	S460	0 0 0 0 0	

2555. $C_{11}H_{22}O_2$
3-Hydroxy-2-propyl-5,5-diethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 186.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2556. $C_{11}H_{22}O_3$
n-Hexyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, hexyl ester
RN: 14144-37-7 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-03	2.999E-01	25	D002	1 2 1 1 0	

2557. $C_{11}H_{22}O_3$
1,3-Dioxolane-4-methanol, 2-hexyl-2-methyl
2-Octanone, cyclic (hydroxymethyl)ethylene acetal
RN: 5660-52-6 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	2.751E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2558. $C_{11}H_{22}O_3$
Octyl lactate
Propanoic acid, 2-hydroxy-, octyl ester
RN: 5464-71-1 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.955E-03	8.000E-01	25	R006	2 2 0 1 0	

2559. $C_{11}H_{22}O_3$
n-Butyl β-*n*-butoxypropionate
Butyl 3-butoxypropionate
Propanoic acid, 3-butoxy-, butyl ester
RN: 14144-48-0 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.951E-03	7.994E-01	25	R034	0 0 0 0 0	

2560. $C_{11}H_{22}O_4$
1,3-Dioxolane-4-methanol, 2-(2-butoxyethyl)-2-methyl
RN: 143458-55-3 **MP** (°C)**:**
MW: 218.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.640E-01	5.763E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2561. $C_{11}H_{23}NOS$
Butylate
S-Ethyl diisobutylthiocarbamate
RN: 2008-41-5 **MP** (°C)**:** <25
MW: 217.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-04	4.500E-02	22	B200	1 0 0 0 1	
2.070E-04	4.500E-02	22	F019	1 0 0 0 1	
1.656E-04	3.599E-02	ns	S460	0 0 0 0 0	
2.070E-04	4.500E-02	rt	M161	0 0 0 0 1	

2562. $C_{11}H_{23}NO_2$
11-Aminoundecanoic acid
Amino-11-undecanoique acide
RN: 2432-99-7 **MP** (°C)**:** 191
MW: 201.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.986E-03	3.998E-01	20	E039	2 0 1 1 1	smoothed
1.600E-03	3.221E-01	30	D051	2 0 0 1 2	
4.962E-03	9.990E-01	30	E039	2 0 1 1 2	smoothed
8.925E-03	1.797E+00	40	E039	2 0 1 1 2	smoothed
1.486E-02	2.991E+00	50	E039	2 0 1 1 2	smoothed
1.000E-02	2.013E+00	60	D051	2 0 0 1 2	
2.471E-02	4.975E+00	60	E039	2 0 1 1 2	smoothed
3.453E-02	6.951E+00	65	E039	2 0 1 1 2	smoothed
4.431E-02	8.920E+00	70	E039	2 0 1 1 2	smoothed
5.405E-02	1.088E+01	75	E039	2 0 1 1 2	smoothed
6.858E-02	1.381E+01	80	E039	2 0 1 1 2	smoothed
8.183E-02	1.647E+01	85	E039	2 0 1 1 2	smoothed
9.740E-02	1.961E+01	90	E039	2 0 1 1 2	smoothed
1.145E-01	2.306E+01	95	E039	2 0 1 1 2	smoothed
1.259E-01	2.534E+01	100	E039	2 0 1 1 2	smoothed

2563. $C_{11}H_{24}$
Undecane
n-Undecane
n-Hendecane
RN: 1120-21-4 **MP** (°C)**:** –26
MW: 156.31 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.60E-06	<1.50E-03	20	M337	2 1 2 2 1	
2.815E-08	4.400E-06	25	M003	1 0 2 2 1	
5.758E-08	9.000E-06	25	T423	0 0 0 0 0	

2564. $C_{12}HCl_7O$
1,2,3,4,6,7,8-Heptachlorodibenzofuran
1,2,3,4,6,7,8-HpCDF
PCDF 131
F 131
RN: 67562-39-4 **MP** (°C)**:** 236
MW: 409.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-12	1.355E-09	22.5	F314	1 1 0 2 2	

2565. $C_{12}HCl_7O_2$
1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin
1,2,3,4,6,7,8-HpCDD
PCDD 73
D 73
Heptachlorodibenzo-*p*-dioxin
RN: 35822-46-9 **MP** (°C)**:** 265
MW: 425.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-12	9.357E-10	7.0	F315	1 2 0 2 2	
2.690E-12	1.144E-09	11.5	F315	1 2 0 2 2	
3.040E-12	1.293E-09	17.0	F315	1 2 0 2 2	
5.400E-12	2.297E-09	21.0	F315	1 2 0 2 2	
6.030E-12	2.565E-09	26.0	F315	1 2 0 2 2	
1.481E-11	6.300E-09	40	F303	1 2 1 2 1	
1.490E-11	6.337E-09	41.0	F315	1 2 0 2 2	

2566. $C_{12}HCl_9$
2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl
2,3,4,5,6,2′,3′,4′,5′-Nonachlorbiphenyl
RN: 40186-72-9 **MP** (°C)**:** 204.5
MW: 464.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-10	7.800E-08	22	O311	2 2 1 2 1	
5.490E-11	2.549E-08	25	D331	2 1 2 2 2	
5.493E-11	2.550E-08	25	D335	1 0 0 0 2	
2.413E-10	1.120E-07	25	W025	1 0 2 2 2	
5.490E-11	2.549E-08	25.0	M324	1 2 1 1 2	
1.100E-10	5.106E-08	32	D331	2 1 2 2 2	
1.100E-10	5.106E-08	32.0	M324	1 2 1 1 2	
1.420E-10	6.592E-08	40	D331	2 1 2 2 2	
1.420E-10	6.592E-08	40.0	M324	1 2 1 1 2	
2.840E-10	1.318E-07	50	D331	2 1 2 2 2	
2.840E-10	1.318E-07	50.0	M324	1 2 1 1 2	

2567. $C_{12}HCl_9$
2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,5′,6,6′-nonachloro-
PCB 208
RN: 52663-77-1 **MP** (°C)**:** 182
MW: 464.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.880E-11	1.801E-08	25	M342	1 0 1 1 2	

2568. $C_{12}H_2Br_8$
Octabromobiphenyl
OBBP
Bromkal 80
RN: 27858-07-7 **MP** (°C)**:** 225.0
MW: 785.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.183E-08	2.500E-05	25	N326	1 0 0 0 1	average

2569. $C_{12}H_2Cl_6O$
1,2,3,6,7,8-Hexachlorodibenzofuran
1,2,3,6,7,8-HxCDF
F 121
PCDF 121
2,3,4,7,8,9-Hexachlorodibenzofuran
RN: 57117-44-9 **MP** (°C)**:** 233
MW: 374.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-11	1.769E-08	22.5	F314	1 1 0 2 2	

2570. $C_{12}H_2Cl_6O$
1,2,3,4,7,8-Hexachlorodibenzofuran
1,2,3,4,7,8-HxCDF
F 118
PCDF 118
RN: 70648-26-9 **MP** (°C)**:** 226
MW: 374.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-11	8.247E-09	22.5	F314	1 1 0 2 2	

2571. $C_{12}H_2Cl_6O_2$
1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin
1,2,3,4,7,8-Hexachlorodibenzo[b,e][1,4]dioxin
1,2,3,4,7,8-Hexachlorodibenzo[1,4]dioxin
1,2,3,4,7,8-HxCDD
D 66
PCDD 66
RN: 39227-28-6 **MP** (°C)**:** 273
MW: 390.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.910E-12	2.310E-09	7.0	F315	1 2 0 2 2	
7.980E-12	3.119E-09	11.5	F315	1 2 0 2 2	
1.070E-11	4.182E-09	17.0	F315	1 2 0 2 2	
1.126E-11	4.400E-09	20	F303	1 2 1 2 1	
1.250E-11	4.886E-09	21.0	F315	1 2 0 2 2	
2.020E-11	7.896E-09	26.0	F315	1 2 0 2 2	
4.861E-11	1.900E-08	40	F303	1 2 1 2 2	
4.860E-11	1.900E-08	41.0	F315	1 2 0 2 2	

2572. $C_{12}H_2Cl_8$
2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl
2,3,4,5,2′,3′,4′,5′-Octachlorbiphenyl
PCB 194
RN: 35694-08-7 **MP** (°C)**:** 156
MW: 429.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.885E-10	1.240E-07	22	O311	2 2 1 2 2	
6.329E-10	2.720E-07	25	W025	1 0 2 2 2	

2573. $C_{12}H_2Cl_8$
2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
2,3,5,6,2′,3′,5′,6′-Octachlorbiphenyl
RN: 2136-99-4 **MP** (°C)**:** 161
MW: 429.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.650E-10	1.139E-07	20	D331	2 1 2 2 2	
2.650E-10	1.139E-07	20.0	M324	1 2 1 1 2	
3.420E-10	1.470E-07	25	D331	2 1 2 2 2	
3.420E-10	1.470E-07	25	D335	1 0 0 0 2	
9.150E-10	3.932E-07	25	M342	1 0 1 1 2	
4.188E-10	1.800E-07	25	W025	1 0 2 2 1	
3.420E-10	1.470E-07	25.0	M324	1 2 1 1 2	
4.930E-10	2.119E-07	32	D331	2 1 2 2 2	
4.930E-10	2.119E-07	32.0	M324	1 2 1 1 2	
1.780E-09	7.650E-07	50	D331	2 1 2 2 2	
1.780E-09	7.650E-07	50.0	M324	1 2 1 1 2	

2574. $C_{12}H_3Cl_5O$
2,3,4,7,8-Pentachlorodibenzofuran
2,3,4,7,8-P5CDF
PeCDF, 2,3,4,7,8-
RN: 57117-31-4 **MP** (°C)**:** 195.5
MW: 340.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-10	2.356E-07	22.5	F314	1 1 0 2 2	

2575. $C_{12}H_3Cl_5O_2$
1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin
Dibenzo[b,e][1,4]dioxin, 1,2,3,4,7-pentachloro-
PCDD 50
RN: 39227-61-7 **MP** (°C)**:** 195
MW: 356.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-10	5.061E-08	7.0	F315	1 2 0 2 2	
1.880E-10	6.701E-08	11.5	F315	1 2 0 2 2	
2.440E-10	8.697E-08	17.0	F315	1 2 0 2 2	
3.367E-10	1.200E-07	20	F303	1 2 1 2 1	
3.450E-10	1.230E-07	21.0	F315	1 2 0 2 2	
4.630E-10	1.650E-07	26.0	F315	1 2 0 2 2	
1.291E-09	4.600E-07	40	F303	1 2 1 2 1	
1.280E-09	4.562E-07	41.0	F315	1 2 0 2 2	

2576. $C_{12}H_3Cl_7$
2,2′,3,3′,4,4′,5-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,4′,5-heptachloro-
PCB 170
CB 170
RN: 35065-30-6 **MP** (°C)**:** 134.5
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.778E-09	3.470E-06	20	M336	2 0 2 2 2	

2577. $C_{12}H_3Cl_7$
2,2′,3,4′,5,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5,5′,6-heptachloro-
PCB 187
RN: 52663-68-0 **MP** (°C)**:** 104
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-08	4.510E-06	20	M336	2 0 2 2 2	

2578. $C_{12}H_3Cl_7$
2,2′,3,3′,5,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5,5′,6-heptachloro-
PCB 178
RN: 52663-67-9 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.840E-06	20	M336	2 0 2 2 2	

2579. $C_{12}H_3Cl_7$
2,2′,3,3′,4,6,6′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,6,6′-heptachloro-
PCB 176
RN: 52663-65-7 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-08	5.850E-06	20	M336	2 0 2 2 2	

2580. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,6-heptachloro-
PCB 173
RN: 68194-16-1 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.052E-08	4.160E-06	20	M336	2 0 2 2 2	

2581. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,6′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,6′-heptachloro-
PCB 174
RN: 38411-25-5 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-08	5.250E-06	20	M336	2 0 2 2 2	

2582. $C_{12}H_3Cl_7$
2,2′,3,4,4′,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5′,6-heptachloro-
PCB 183
RN: 52663-69-1 **MP** (°C)**:** 83
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-08	4.900E-06	20	M336	2 0 2 2 2	

2583. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5′,6-heptachloro-
PCB 175
RN: 40186-70-7 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E-08	8.940E-06	20	M336	2 0 2 2 2	

2584. $C_{12}H_3Cl_7$
2,2′,3,3′,4,4′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,4′,6-heptachloro-
PCB 171
RN: 52663-71-5 **MP** (°C)**:** 117
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-08	4.120E-06	20	M336	2 0 2 2 2	
5.490E-09	2.170E-06	25	M342	1 0 1 1 2	
5.490E-09	2.170E-06	ns	M308	0 0 1 1 2	

2585. $C_{12}H_3Cl_7$
2,2′,3,3′,4′,5,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5′,6′-heptachloro-
PCB 177
RN: 52663-70-4 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.219E-08	4.820E-06	20	M336	2 0 2 2 2	

2586. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,5′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,5′-heptachloro-
PCB 172
RN: 52663-74-8 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-08	4.300E-06	20	M336	2 0 2 2 2	

2587. $C_{12}H_3Cl_7$
2,2′,3,4,4′,5,5′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5,5′-heptachloro-
PCB 180
RN: 35065-29-3 **MP** (°C)**:** 112
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.739E-09	3.850E-06	20	M336	2 0 2 2 2	

2588. $C_{12}H_3Cl_7$
Heptachlorobiphenyl
1,1′-Biphenyl, heptachloro-
Heptachlorodiphenyl
RN: 28655-71-2 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-08	6.250E-06	11.5	D085	0 0 0 0 0	mixed isomers

2589. $C_{12}H_3Cl_7$
2,2′,3,4,5,5′,6-Heptachlorobiphenyl
2,3,4,5,6,2′,5′-Heptachlorbiphenyl
PCB 185
RN: 52712-05-7 **MP** (°C)**:** 147
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-08	5.460E-06	20	M336	2 0 2 2 2	*sic*
1.189E-09	4.700E-07	25	W025	1 0 2 2 1	

2590. $C_{12}H_4Br_6$
FireMaster FF-1 (hexabromobiphenyl mixture)
RN: **MP** (°C)**:**
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2591. $C_{12}H_4Br_6$
2,2′,4,4′,6,6′-Hexabromobiphenyl
Hexabromobiphenyl
Polybromilated biphenyl
RN: 36355-01-8 **MP** (°C)**:** 72
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.954E-04	6.247E-01	26.5	G312	0 0 0 0 0	

2592. $C_{12}H_4Br_6$
Fire Master BP-6 (hexabromophenyl mixture)
RN: 59536-65-1 **MP** (°C)**:**
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2593. $C_{12}H_4Br_6O$
2,2′,4,4′,5,5′-Hexabromodiphenylether
RN: **MP** (°C)**:**
MW: 643.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.723E-11	3.040E-08	10	K431	0 0 0 0 0	
7.831E-11	5.040E-08	25	K431	0 0 0 0 0	
1.896E-10	1.220E-07	35	K431	0 0 0 0 0	

2594. $C_{12}H_4Cl_4O$
2,3,7,8-Tetrachlorodibenzofuran
2,3,7,8-T4CDF
RN: 51207-31-9 **MP** (°C)**:** 227
MW: 305.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-09	4.192E-07	22.5	F314	1 1 0 2 2	

2595. $C_{12}H_4Cl_4O_2$

1,2,3,4-Tetrachlorodibenzo-*p*-dioxin
1,2,3,4-TCDD
1,2,3,4-Tetrachlorodibenzo[b,e][1,4]dioxin
RN: 30746-58-8 **MP** (°C)**:** 184–186
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-10	1.130E-07	4.0	D330	2 2 1 2 2	
4.007E-11	1.290E-08	4.3	L321	2 0 2 2 2	
1.065E-09	3.430E-07	5	S352	2 2 0 2 2	
1.401E-09	4.510E-07	15	S352	2 2 0 2 2	
1.500E-09	4.830E-07	17.3	L321	2 0 2 2 2	
1.708E-09	5.500E-07	25	S352	2 2 0 2 1	average of 2
1.957E-09	6.300E-07	25	S352	2 2 0 2 1	
1.460E-09	4.701E-07	25.0	D330	2 2 1 2 2	
3.541E-09	1.140E-06	35	S352	2 2 0 2 2	
3.630E-09	1.169E-06	40.0	D330	2 2 1 2 2	
6.476E-09	2.085E-06	45	S352	2 2 0 2 2	

2596. $C_{12}H_4Cl_4O_2$

2,3,7,8-Tetrachlorodibenzo-*p*-dioxin
TCDD
2,3,7,8-Tetrachlorodibenzodioxin
RN: 1746-01-6 **MP** (°C)**:** 310
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-11	1.930E-08	22	M340	1 2 2 1 2	
6.212E-10	2.000E-07	ns	C098	0 0 0 0 0	
6.212E-10	2.000E-07	ns	K138	0 0 0 0 2	
6.212E-10	2.000E-07	ns	N320	0 0 0 0 0	
2.457E-11	7.910E-09	rt	A323	0 2 2 1 2	

2597. $C_{12}H_4Cl_4O_2$

1,3,6,8-Tetrachlorodibenzo-*p*-dioxin
PCDD 42
1,3,6,8-Tetrachlorodibenzo[1,4]dioxin
RN: 33423-92-6 **MP** (°C)**:** 219
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.939E-10	3.200E-07	20	F303	1 2 1 2 1	
9.939E-10	3.200E-07	20	W319	1 2 1 2 1	
1.211E-09	3.900E-07	40	F303	1 2 1 2 1	
1.211E-09	3.900E-07	40	W319	1 2 1 2 1	
9.845E-10	3.170E-07	ns	W332	0 1 0 2 2	

2598. $C_{12}H_4Cl_4O_2$
1,2,3,7-Tetrachlorodibenzo-*p*-dioxin
PCDD 29
RN: 67028-18-6 **MP** (°C)**:** 175
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.560E-10	2.434E-07	7.0	F315	1 2 0 2 2	
8.120E-10	2.614E-07	11.5	F315	1 2 0 2 2	
1.250E-09	4.025E-07	17.0	F315	1 2 0 2 2	
1.336E-09	4.300E-07	20	F303	1 2 1 2 1	
1.490E-09	4.797E-07	21.0	F315	1 2 0 2 2	
2.260E-09	7.277E-07	26.0	F315	1 2 0 2 2	
3.944E-09	1.270E-06	40	F303	1 2 1 2 1	
4.330E-09	1.394E-06	41.0	F315	1 2 0 2 2	

2599. $C_{12}H_4Cl_6$
2,2′,3,4′,5,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5,5′-hexachloro-
PCB 146
RN: 51908-16-8 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.103E-08	7.590E-06	20	M336	2 0 2 2 2	

2600. $C_{12}H_4Cl_6$
2,2′,3,3′,4,4′-Hexachlorobiphenyl
2,3,4,2′,3′,4′-Hexachlorbiphenyl
PCB 128
1,1′-Biphenyl, 2,2′,3,3′,4,4′-hexachloro-
RN: 38380-07-3 **MP** (°C)**:** 150
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-08	6.700E-06	20	M336	2 0 2 2 2	*sic*
9.690E-10	3.497E-07	25	D306	2 1 2 2 2	
7.840E-10	2.829E-07	25	M342	1 0 1 1 2	
1.219E-09	4.400E-07	25	W025	1 0 2 2 1	

2601. $C_{12}H_4Cl_6$
2,2′,3,3′,4,5-Hexachlorobiphenyl
2,3,4,5,2′,3′-Hexachlorbiphenyl
2,2′,3,3′,4,5′-Hexachlorobiphenyl
PCB 129
RN: 55215-18-4 **MP** (°C)**:** 101
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-08	5.690E-06	20	M336	2 0 2 2 2	
1.610E-08	5.810E-06	25	D306	2 1 2 2 2	
2.355E-09	8.500E-07	25	W025	1 0 2 2 1	

2602. $C_{12}H_4Cl_6$
2,3,3′,4,4′,5′-Hexachlorobiphenyl
2,3,3′,4,4′,5-Hexachlorobiphenyl
RN: 38380-08-4 **MP** (°C)**:** 127
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-08	5.330E-06	20	M336	2 0 2 2 2	

2603. $C_{12}H_4Cl_6$
2,2′,3,3′,6,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,6,6′-hexachloro-, (+)-
(+)-PCB 136
RN: 207004-30-6 **MP** (°C)**:** 114
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.050E-09	1.101E-06	4	D331	2 1 2 2 2	
3.050E-09	1.101E-06	4.0	M324	1 2 1 1 2	
9.010E-09	3.252E-06	20	D331	2 1 2 2 2	
5.586E-08	2.016E-05	20	M336	2 0 2 2 2	
9.010E-09	3.252E-06	20.0	M324	1 2 1 1 2	
1.250E-08	4.511E-06	25	D331	2 1 2 2 2	
1.250E-08	4.510E-06	25	D335	1 0 0 0 2	
1.670E-08	6.027E-06	25	M342	1 0 1 1 2	
1.250E-08	4.511E-06	25.0	M324	1 2 1 1 2	
1.850E-08	6.676E-06	32	D331	2 1 2 2 2	
1.850E-08	6.676E-06	32.0	M324	1 2 1 1 2	
1.670E-08	6.027E-06	ns	M308	0 0 1 1 2	

2604. $C_{12}H_4Cl_6$
2,2′,3,3′,5,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5,6′-hexachloro-
PCB 135
RN: 52744-13-5 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2605. $C_{12}H_4Cl_6$
2,3,3′,4′,5,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5,6-hexachloro-
PCB 163
RN: 74472-44-9 **MP** (°C)**:** 122
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-08	5.300E-06	25	B319	2 0 1 2 1	
1.471E-08	5.310E-06	25	H341	1 0 0 0 2	

2606. $C_{12}H_4Cl_6$
2,3,3′,4,4′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4,4′,6-hexachloro-
PCB 158
RN: 74472-42-7 **MP** (°C)**:** 107
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.070E-06	20	M336	2 0 2 2 2	

2607. $C_{12}H_4Cl_6$
Hexachlorobiphenyl
1,1′-Biphenyl, hexachloro-
RN: 26601-64-9 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.754E-08	9.940E-06	11.5	D085	0 0 0 0 0	mixed isomers

2608. $C_{12}H_4Cl_6$
Aroclor 1260
Arochlor 1260
RN: 11096-82-5 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:** 402.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.879E-08	1.400E-05	4	M336	2 0 2 2 1	
3.990E-08	1.440E-05	20	M336	2 0 2 2 2	
6.927E-08	2.500E-05	20	N326	1 0 0 0 1	

2609. $C_{12}H_4Cl_6$
2,2′,3,5,5′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5,5′,6-hexachloro-
PCB 151
RN: 52663-63-5 **MP** (°C)**:** 100
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-08	1.355E-05	20	M336	2 0 2 2 2	

2610. $C_{12}H_4Cl_6$
2,2′,3,3′,4,6-Hexachlorobiphenyl
2,2′,3,4′,5′,6′-Hexachlorobiphenyl
PCB 131
RN: 61798-70-7 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.358E-08	1.212E-05	20	M336	2 0 2 2 2	

2611. $C_{12}H_4Cl_6$
2,2′,3,3′,5,6-Hexachlorobiphenyl
2,3,5,6,2′,3′-Hexachlorbiphenyl
RN: 52704-70-8 **MP** (°C)**:** 132
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-08	1.295E-05	20	M336	2 0 2 2 2	*sic*
2.522E-09	9.100E-07	25	W025	1 0 2 2 1	

2612. $C_{12}H_4Cl_6$
2,2′,3,4,5,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,5,5′-hexachloro-
PCB 141
RN: 52712-04-6 **MP** (°C)**:** 85
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.092E-08	7.550E-06	20	M336	2 0 2 2 2	

2613. $C_{12}H_4Cl_6$
2,2′,3,4,5′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,5′,6-hexachloro-
PCB 144
RN: 68194-14-9 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2614. $C_{12}H_4Cl_6$
2,2′,4,4′,5,5′-Hexachlorobiphenyl
2,4,5,2′,4′,5′-PCB
2,4,5,2′,4′,5′-Hexachlorobiphenyl
PCB 129
PCB 153
RN: 35065-27-1 **MP** (°C)**:** 103
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-08	4.619E-06	4.0	D330	2 2 1 2 2	
2.533E-08	9.140E-06	20	M336	2 0 2 2 2	*sic*
7.759E-09	2.800E-06	22	C413	2 0 2 2 1	
3.187E-09	1.150E-06	22	O311	2 2 1 2 2	
2.632E-09	9.500E-07	24	C053	0 0 0 0 0	
2.632E-09	9.500E-07	24	F071	1 1 2 1 1	
2.632E-09	9.500E-07	24	M344	1 0 0 0 1	
2.390E-09	8.625E-07	25	D306	2 1 2 2 2	
3.325E-09	1.200E-06	25	W025	1 0 2 2 1	
2.340E-08	8.445E-06	25.0	D330	2 2 1 2 2	
3.540E-08	1.278E-05	40	D330	2 2 1 2 2	
2.641E-09	9.530E-07	ns	H058	0 1 2 1 2	

2615. $C_{12}H_4Cl_6$
2,2′,3,4,4′,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5′-hexachloro-
PCB 138
CB 138
K 138
RN: 35065-28-2 **MP** (°C)**:** 80.5
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.020E-08	7.290E-06	20	M336	2 0 2 2 2	

2616. $C_{12}H_4Cl_6$
2,2′,3,4,4′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,6-hexachloro-
PCB 139
RN: 56030-56-9 **MP** (°C)**:** 73
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.372E-08	1.217E-05	20	M336	2 0 2 2 2	

2617. $C_{12}H_4Cl_6$
2,2′,3,4,4′,5-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5-hexachloro-
PCB 137
RN: 35694-06-5 **MP** (°C)**:** 77
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-08	8.400E-06	20	M336	2 0 2 2 2	

2618. $C_{12}H_4Cl_6$
2,2′,4,4′,6,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′,6,6′-hexachloro-
PCB 155
RN: 33979-03-2 **MP** (°C)**:** 112.5
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-09	1.090E-06	22	O311	2 2 1 2 2	
6.280E-09	2.266E-06	25	D306	2 1 2 2 2	
9.120E-09	3.291E-06	25	L322	1 1 2 2 2	
1.130E-09	4.078E-07	25	M342	1 0 1 1 2	
2.494E-09	9.000E-07	25	W025	1 0 2 2 1	
1.130E-09	4.078E-07	ns	M308	0 0 1 1 2	

2619. $C_{12}H_5Br_5$
2,2′,4,5,5′-Pentabromobiphenyl
1,1′-Biphenyl, 2,2′,4,5,5′-pentabromo-
PBB 101
RN: 67888-96-4 **MP** (°C)**:**
MW: 548.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-10	1.032E-07	4.0	D330	2 2 1 2 2	
8.060E-10	4.423E-07	25	D330	2 2 1 2 2	
1.790E-09	9.822E-07	40.0	D330	2 2 1 2 2	

2620. $C_{12}H_5Br_5O$
2,2′,4,4′,5-Pentabromodiphenyl ether
RN: **MP** (°C)**:**
MW: 564.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.108E-09	2.320E-06	10	K431	0 0 0 0 0	
7.738E-09	4.370E-06	25	K431	0 0 0 0 0	
1.186E-08	6.700E-06	35	K431	0 0 0 0 0	

2621. $C_{12}H_5Cl_3O_2$
1,2,4-Trichlorodibenzo-*p*-dioxin
Dibenzo[b,e][1,4]dioxin, 1,2,4-trichloro-
PCDD 14
RN: 39227-58-2 **MP** (°C)**:** 129
MW: 287.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.617E-09	2.190E-06	5	S352	2 2 0 2 2	
1.659E-08	4.770E-06	15	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
5.801E-08	1.668E-05	35	S352	2 2 0 2 2	
9.815E-08	2.822E-05	45	S352	2 2 0 2 2	

2622. $C_{12}H_5Cl_5$
2,2′,3,4,4′-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′-pentachloro-
PCB 85
RN: 65510-45-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.712E-08	2.191E-05	20	M336	2 0 2 2 2	

2623. $C_{12}H_5Cl_5$
2,2′,3,4′,6-Pentachlorobiphenyl
2,2′,4,6,6′-Pentachlorobiphenyl
PCB 104
RN: 56558-16-8 **MP** (°C)**:** 85
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-07	3.945E-05	20	M336	2 0 2 2 2	
4.770E-08	1.557E-05	25	D306	2 1 2 2 2	

2624. $C_{12}H_5Cl_5$
2,2′,3,3′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,6-pentachloro-
PCB 84
RN: 52663-60-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-07	4.702E-05	20	M336	2 0 2 2 2	

2625. $C_{12}H_5Cl_5$
2,2′,3,3′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5-pentachloro-
PCB 83
RN: 60145-20-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.648E-08	2.823E-05	20	M336	2 0 2 2 2	

2626. $C_{12}H_5Cl_5$
2′,3,4,5,5′-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5,5′-pentachloro-
PCB 124
RN: 70424-70-3 **MP** (°C)**:** 105
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-08	1.581E-05	20	M336	2 0 2 2 2	

2627. $C_{12}H_5Cl_5$
2,2′,3′,4,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5′-pentachloro-
PCB 87
RN: 41464-51-1 **MP** (°C)**:** 81
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.703E-08	2.841E-05	20	M336	2 0 2 2 2	

2628. $C_{12}H_5Cl_5$
2,2′,3,4,5′-Pentachlorobiphenyl
2,3,4,2′,5′-Pentachlorbiphenyl
PCB 87
RN: 38380-02-8 **MP** (°C)**:** 112
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.009E-08	2.941E-05	20	M336	2 0 2 2 2	
1.379E-08	4.500E-06	25	W025	1 0 2 2 1	

2629. $C_{12}H_5Cl_5$
2,3,3′,4′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,6-pentachloro-
PCB 110
RN: 38380-03-9 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.829E-08	2.882E-05	20	M336	2 0 2 2 2	

2630. $C_{12}H_5Cl_5$
2′,3,3′,4,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5′-pentachloro-
PCB 122
RN: 76842-07-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.933E-08	1.284E-05	20	M336	2 0 2 2 2	

2631. $C_{12}H_5Cl_5$
2,2′,3,3′,4-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4-pentachloro-
PCB 82
RN: 52663-62-4 **MP** (°C)**:** 119
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.908E-08	2.908E-05	20	M336	2 0 2 2 2	

2632. $C_{12}H_5Cl_5$
2,2′,3,4,5-Pentachlorobiphenyl
2,3,4,5,2′-Pentachlorbiphenyl
PCB 86
RN: 55312-69-1 **MP** (°C)**:** 112
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.046E-08	2.300E-05	23	W024	0 0 0 0 0	
1.042E-07	3.400E-05	25	B319	2 0 1 2 1	
1.069E-07	3.490E-05	25	H341	1 0 0 0 2	
3.002E-08	9.800E-06	25	W025	1 0 2 2 2	

2633. $C_{12}H_5Cl_5$
2,2′,3,4,6-Pentachlorobiphenyl
2,3,4,6,2′-Pentachlorbiphenyl
PCB 88
RN: 55215-17-3 **MP** (°C)**:** 63
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.676E-08	1.200E-05	25	W025	1 0 2 2 2	

2634. $C_{12}H_5Cl_5$
2,2′,3,5′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5′,6-pentachloro-
PCB 95
RN: 38379-99-6 **MP** (°C)**:** 94
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-07	5.413E-05	20	M336	2 0 2 2 2	

2635. $C_{12}H_5Cl_5$
2,2′,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′,5-pentachloro-
PCB 99
RN: 38380-01-7 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.798E-08	2.219E-05	20	M336	2 0 2 2 2	

2636. $C_{12}H_5Cl_5$
2,3′,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,4′,5-pentachloro-
PCB 118
CB 118
RN: 31508-00-6 **MP** (°C)**:** 109
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.117E-08	1.344E-05	20	M336	2 0 2 2 2	

2637. $C_{12}H_5Cl_5$
2,3,3′,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5-pentachloro-
PCB 107
RN: 70424-68-9 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.546E-08	1.484E-05	20	M336	2 0 2 2 2	

2638. $C_{12}H_5Cl_5$
2,3,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,4,4′,5-pentachloro-
PCB 114
RN: 74472-37-0 **MP** (°C)**:** 98
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-08	1.598E-05	20	M336	2 0 2 2 2	

2639. $C_{12}H_5Cl_5$
2,3,4,5,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,4,5,6-pentachloro-
PCB 116
RN: 18259-05-7 **MP** (°C)**:** 123
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.166E-08	1.360E-05	22	O311	2 2 1 2 2	
1.230E-08	4.015E-06	25	D306	2 1 2 2 2	
1.680E-08	5.484E-06	25	M342	1 0 1 1 2	
2.083E-08	6.800E-06	25	W025	1 0 2 2 1	
1.680E-08	5.484E-06	ns	M308	0 0 1 1 2	

2640. $C_{12}H_5Cl_5$
2,2′,4,5,5′-Pentachlorobiphenyl
2,4,5,2′,5′-PCB
2,2′,4,5,5′-PCB
RN: 37680-73-2 **MP** (°C)**:** 77
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-08	6.137E-06	4	D331	2 1 2 2 2	
1.880E-08	6.137E-06	4.0	M324	1 2 1 1 2	
3.710E-08	1.211E-05	20	D331	2 1 2 2 2	
8.044E-08	2.626E-05	20	M336	2 0 2 2 2	
3.710E-08	1.211E-05	20.0	M324	1 2 1 1 2	
3.063E-08	1.000E-05	24	C053	0 0 0 0 0	
3.370E-08	1.100E-05	24	C311	0 0 0 0 0	EFG
3.063E-08	1.000E-05	24	F071	1 1 2 1 1	
3.063E-08	1.000E-05	24	M344	1 0 0 0 1	
3.370E-08	1.100E-05	25	C313	0 0 0 0 0	
2.070E-08	6.757E-06	25	D306	2 1 2 2 2	
4.720E-08	1.541E-05	25	D331	2 1 2 2 2	
4.718E-08	1.540E-05	25	D335	1 0 0 0 2	
5.920E-08	1.933E-05	25	M342	1 0 1 1 2	
1.287E-08	4.200E-06	25	W025	1 0 2 2 1	
4.720E-08	1.541E-05	25.0	M324	1 2 1 1 2	
6.830E-08	2.230E-05	32	D331	2 1 2 2 2	
6.830E-08	2.230E-05	32.0	M324	1 2 1 1 2	
3.155E-08	1.030E-05	ns	H058	0 1 2 1 2	
5.820E-08	1.900E-05	ns	M118	0 1 1 1 1	
5.920E-08	1.933E-05	ns	M308	0 0 1 1 2	

2641. $C_{12}H_5Cl_5$
Pentachlorobiphenyl
2,2′,4,4′,6-Pentachlorobiphenyl
Kanekrol 500
RN: 25429-29-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.341E-08	2.070E-05	11.5	D085	0 0 0 0 0	mixed isomers
9.496E-08	3.100E-05	22.5	G301	0 0 0 0 0	

2642. $C_{12}H_5N_5O_{11}$
Pentanitrophenylether
Benzene, 2-(2,4-dinitrophenoxy)-1,3,5-trinitro-
RN: 5950-87-8 **MP** (°C)**:**
MW: 395.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.771E-04	7.000E-02	27	D067	1 2 0 0 0	
4.302E-04	1.700E-01	50	D067	1 2 0 0 1	
2.404E-03	9.500E-01	100	D067	1 2 0 0 1	

2643. $C_{12}H_5N_7O_{12}$
Hexanitrodiphenylamine
Benzenamine, 2,4,6-trinitro-*N*-(2,4,6-trinitrophenyl)-
RN: 131-73-7 **MP** (°C)**:**
MW: 439.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E-04	6.000E-02	17	D070	1 2 0 0 0	
4.325E-04	1.900E-01	50	D070	1 2 0 0 1	
7.738E-04	3.399E-01	100	D070	1 2 0 0 1	

2644. $C_{12}H_6Br_4$
2,2′,5,5′-Tetrabromobiphenyl
Tetrabromobiphenyl
RN: 59080-37-4 **MP** (°C)**:** 143
MW: 469.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-03	4.054E+00	26.5	G312	0 0 0 0 0	

2645. $C_{12}H_6Br_4O$
2,2′,4,4′-Tetrabromodiphenylether
RN: **MP** (°C)**:**
MW: 485.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.661E-08	8.070E-06	10	K431	0 0 0 0 0	
3.026E-08	1.470E-05	25	K431	0 0 0 0 0	
5.105E-09	2.480E-06	35	K431	0 0 0 0 0	

2646. $C_{12}H_6Cl_2O_2$
2,7-Dichlorodibenzo-*p*-dioxin
2,7-DCDD
2,8-Dichlorodibenzodioxin
RN: 33857-26-0 **MP** (°C)**:** 201
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.307E-09	1.090E-06	5	S352	2 2 0 2 2	
7.942E-09	2.010E-06	15	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
2.873E-08	7.270E-06	35	S352	2 2 0 2 2	
5.295E-08	1.340E-05	45	S352	2 2 0 2 2	

2647. $C_{12}H_6Cl_2O_2$
2,8-Dichlorodibenzo-*p*-dioxin
2,8-Dichlorodibenzodioxin
PCDD 12
3,6-Dichloro-9,10-dioxaanthracene
RN: 38964-22-6 **MP** (°C)**:** 151
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.746E-08	4.420E-06	5	S352	2 2 0 2 2	
3.394E-08	8.590E-06	15	S352	2 2 0 2 2	
6.599E-08	1.670E-05	25	S352	2 2 0 2 2	
6.614E-08	1.674E-05	25	S352	2 2 0 2 2	
1.088E-07	2.753E-05	35	S352	2 2 0 2 2	
2.035E-07	5.150E-05	45	S352	2 2 0 2 2	

2648. $C_{12}H_6Cl_2O_2$
2,3-Dichlorodibenzo-*p*-dioxin
2,3-Dichlorodibenzodioxin
PCDD 10
RN: 29446-15-9 **MP** (°C)**:** 160
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.454E-08	3.680E-06	5	S352	2 2 0 2 2	
2.829E-08	7.160E-06	15	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
1.201E-07	3.040E-05	35	S352	2 2 0 2 2	
2.315E-07	5.860E-05	45	S352	2 2 0 2 2	

2649. $C_{12}H_6Cl_3NO_3$
Quinonamid
2-(Dichloroacetamido)-3-chloro-1,4-naphthoquinone
HOE 13465OH
Chinonamid
2-[(Dichloroacetyl)amino]-3-chloro-1,4-naphthoquinone
RN: 27541-88-4 **MP** (°C)**:** 212.5
MW: 318.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-06	3.000E-03	23	M161	1 0 0 0 0	pH 4.6

2650. $C_{12}H_6Cl_3NO_3$
Chlornitrofen
4-Nitrophenyl 2,4,6-trichlorophenyl ether
1,3,5-Trichloro-2-(4-nitrophenoxy)benzene
1′,3′,5′-Trichlorophenyl-4-nitrophenyl ether
RN: 1836-77-7 **MP** (°C)**:**
MW: 318.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E-06	7.640E-04	22	K137	1 1 2 1 0	

2651. $C_{12}H_6Cl_4$
2,2′,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,5-tetrachloro-
PCB 48
RN: 70362-47-9 **MP** (°C)**:** 63.9
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-07	2.995E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	25	M342	1 0 1 1 2	

2652. $C_{12}H_6Cl_4$
2,3′,4,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,6-tetrachloro-
PCB 69
RN: 60233-24-1 **MP** (°C)**:** 46
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.004E-08	2.045E-05	20	M336	2 0 2 2 2	

2653. $C_{12}H_6Cl_4$
Aroclor 1254
Arochlor 1254
RN: 11097-69-1 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-07	3.900E-05	4	M336	2 0 2 2 1	
8.288E-08	2.420E-05	11.5	D085	0 0 0 0 0	
9.623E-08	2.810E-05	16.50	W033	1 0 2 2 2	
8.459E-08	2.470E-05	16.50	W033	1 0 2 2 2	
1.473E-07	4.300E-05	20	M336	2 0 2 2 1	
1.712E-07	5.000E-05	20	N326	1 0 0 0 1	
~1.92E-07	~5.60E-05	ns	H117	0 2 2 2 0	
1.541E-07	4.500E-05	ns	L106	0 0 2 1 1	
1.370E-07	4.000E-05	ns	M184	0 0 0 0 0	

2654. $C_{12}H_6Cl_4$
Aroclor 1248
Arochlor 1248
RN: 12672-29-6 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:** 357.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.425E-07	1.000E-04	20	N326	1 0 0 0 2	

2655. $C_{12}H_6Cl_4$
3,3′,5,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 3,3′,5,5′-tetrachloro-
PCB 80
RN: 33284-52-5 **MP** (°C)**:** 164
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.220E-09	1.232E-06	25	D306	2 1 2 2 2	

2656. $C_{12}H_6Cl_4$
3,3′,4,4′-Tetrachlorobiphenyl
3,4,3′,4′-Tetrachlorbiphenyl
RN: 32598-13-3 **MP** (°C)**:** 183
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-10	1.460E-07	4	D331	2 1 2 2 2	
5.000E-10	1.460E-07	4.0	M324	1 2 1 1 2	
1.490E-09	4.351E-07	20	D331	2 1 2 2 2	
1.490E-09	4.351E-07	20.0	M324	1 2 1 1 2	
6.165E-09	1.800E-06	22	O311	2 2 1 2 1	
1.404E-07	4.100E-05	23	W024	0 0 0 0 0	*sic*
1.880E-09	5.489E-07	25	D306	2 1 2 2 2	
1.950E-09	5.694E-07	25	D331	2 1 2 2 2	
1.949E-09	5.690E-07	25	D335	1 0 0 0 2	
2.569E-09	7.500E-07	25	W025	1 0 2 2 1	
1.950E-09	5.694E-07	25.0	M324	1 2 1 1 2	
4.040E-09	1.180E-06	32	D331	2 1 2 2 2	
4.040E-09	1.180E-06	32.0	M324	1 2 1 1 2	

2657. $C_{12}H_6Cl_4$
2,4,4′,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,4,4′,6-tetrachloro-
PCB 75
RN: 32598-12-2 **MP** (°C)**:** 65
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	9.110E-05	25	D306	2 1 2 2 2	

2658. $C_{12}H_6Cl_4$
2,4,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,4,4′,5-tetrachloro-
PCB 74
RN: 32690-93-0 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.049E-07	3.064E-05	20	M336	2 0 2 2 2	

2659. $C_{12}H_6Cl_4$
2,3,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4,5-tetrachloro-
PCB 61
RN: 33284-53-6 **MP** (°C)**:** 92
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.390E-08	9.900E-06	25	B319	2 0 1 2 1	
4.780E-08	1.396E-05	25	D306	2 1 2 2 2	
4.677E-08	1.366E-05	25	L322	1 1 2 2 2	
7.170E-08	2.094E-05	25	M342	1 0 1 1 2	
6.575E-08	1.920E-05	25	W025	1 0 2 2 2	
7.170E-08	2.094E-05	ns	M308	0 0 1 1 2	

2660. $C_{12}H_6Cl_4$
2,3,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4,4′-tetrachloro-
PCB 60
RN: 33025-41-1 **MP** (°C)**:** 142
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-07	3.893E-05	20	M336	2 0 2 2 2	

2661. $C_{12}H_6Cl_4$
2,3,4′,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4′,6-tetrachloro-
PCB 64
RN: 52663-58-8 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.207E-07	9.365E-05	20	M336	2 0 2 2 2	

2662. $C_{12}H_6Cl_4$
2,3,3′,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′-tetrachloro-
PCB 56
RN: 41464-43-1 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-07	3.894E-05	20	M336	2 0 2 2 2	

2663. $C_{12}H_6Cl_4$
2,3′,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,4′-tetrachloro-
PCB 66
RN: 32598-10-0 **MP** (°C)**:** 128.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.676E-05	20	M336	2 0 2 2 2	

2664. $C_{12}H_6Cl_4$
2,3′,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5-tetrachloro-
PCB 70
RN: 32598-11-1 **MP** (°C)**:** 106
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-07	3.618E-05	20	M336	2 0 2 2 2	
2.055E-07	6.000E-05	23	W024	0 0 0 0 0	
7.534E-08	2.200E-05	ns	B301	0 2 1 1 1	

2665. $C_{12}H_6Cl_4$
2,2′,6,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,6,6′-tetrachloro-
PCB 54
RN: 15968-05-5 **MP** (°C)**:** 198.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-09	2.700E-06	22	O311	2 2 1 2 1	
4.070E-08	1.188E-05	25	D306	2 1 2 2 2	

2666. $C_{12}H_6Cl_4$
2,2′,5,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,5,5′-tetrachloro-
PCB 52
RN: 35693-99-3 **MP** (°C)**:** 87
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.855E-07	1.126E-04	20	M336	2 0 2 2 2	
5.240E-08	1.530E-05	22	O311	2 2 1 2 2	
1.575E-07	4.600E-05	23	W024	0 0 0 0 0	
5.822E-07	1.700E-04	25	B319	2 0 1 2 2	
3.750E-07	1.095E-04	25	D306	2 1 2 2 2	
1.250E-07	3.650E-05	25	H341	1 0 0 0 2	
1.884E-07	5.500E-05	ns	B301	0 2 1 1 1	
9.076E-08	2.650E-05	ns	H058	0 1 2 1 2	
5.480E-08	1.600E-05	ns	M118	0 1 1 1 1	

2667. $C_{12}H_6Cl_4$
2,2′,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′-tetrachloro-
PCB 47
RN: 2437-79-8 **MP** (°C)**:** 42.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-07	6.600E-05	22	C413	2 0 2 2 1	
1.853E-07	5.410E-05	22	O311	2 2 1 2 2	
5.993E-07	1.750E-04	23	W024	0 0 0 0 0	
7.534E-07	2.200E-04	25	B351	1 0 0 1 1	

2668. $C_{12}H_6Cl_4$
2,3,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4′,5-tetrachloro-
PCB 63
RN: 74472-34-7 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.997E-08	2.627E-05	20	M336	2 0 2 2 2	

2669. $C_{12}H_6Cl_4$
2,2′,5,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,5,6′-tetrachloro-
PCB 53
RN: 41464-41-9 **MP** (°C)**:** 103
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-07	1.085E-04	20	M336	2 0 2 2 2	
1.630E-07	4.759E-05	25	D306	2 1 2 2 2	

2670. $C_{12}H_6Cl_4$
2,2′,3,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5′-tetrachloro-
PCB 44
RN: 41464-39-5 **MP** (°C)**:** 47
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.426E-07	1.001E-04	20	M336	2 0 2 2 2	
2.226E-07	6.500E-05	23	W024	0 0 0 0 0	
2.740E-07	8.000E-05	25	B319	2 0 1 2 0	

2671. $C_{12}H_6Cl_4$
2,2′,3,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′-tetrachloro-
PCB 42
RN: 36559-22-5 **MP** (°C)**:** 68
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-07	6.083E-05	20	M336	2 0 2 2 2	

2672. $C_{12}H_6Cl_4$
2,2′,3,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,6′-tetrachloro-
PCB 46
RN: 41464-47-5 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E-07	1.059E-04	20	M336	2 0 2 2 2	

2673. $C_{12}H_6Cl_4$
Tetrachlorobiphenyl
1,1′-Biphenyl, tetrachloro-
Pyralene 1498
RN: 26914-33-0 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.825E-07	5.330E-05	11.5	D085	0 0 0 0 0	mixed isomers

2674. $C_{12}H_6Cl_4$
2′,3,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5′-tetrachloro-
PCB 76
RN: 70362-48-0 **MP** (°C)**:** 92.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-07	5.513E-05	20	M336	2 0 2 2 2	

2675. $C_{12}H_6Cl_4$
2,2′,3,4-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4-tetrachloro-
PCB 41
RN: 52663-59-9 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-07	6.480E-05	20	M336	2 0 2 2 2	

2676. $C_{12}H_6Cl_4$
2,2′,4,5′-Tetrachlorobiphenyl
2,2′,4′,5-Tetrachlorobiphenyl
PCB 49
RN: 41464-40-8 **MP** (°C)**:** 67
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.676E-07	7.814E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	ns	M308	0 0 1 1 2	

2677. $C_{12}H_6Cl_4$
2,2′,3,3′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′-tetrachloro-
PCB 40
RN: 38444-93-8 **MP** (°C)**:** 121.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.764E-07	8.070E-05	20	M336	2 0 2 2 2	
5.822E-07	1.700E-04	23	W024	0 0 0 0 0	
5.340E-08	1.559E-05	25	D306	2 1 2 2 2	

2678. $C_{12}H_6Cl_4O_2S$
Tetradifon
2,4,5,4′-Tetrachlorodiphenyl sulfone
Tedion
Aracnol K
Akaritox
Rotetra
RN: 116-29-0 **MP** (°C)**:** 148.5
MW: 356.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.404E-07	5.000E-05	10	V301	1 0 0 0 0	
5.617E-04	2.000E-01	50	M161	1 0 0 0 0	
9.549E-07	3.400E-04	50	V301	1 0 0 0 1	

2679. $C_{12}H_7BrClNO_2$
Halacrinate
7-Bromo-5-chloro-8-quinolinyl 2-propenoate
Halocrinate
RN: 34462-96-9 **MP** (°C)**:** 100.5
MW: 312.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	6.000E-03	20	M161	1 0 0 0 0	

2680. $C_{12}H_7ClO_2$
1-Chlorodibenzo-*p*-dioxin
1-Monochlorodibenzodioxin
PCDD 1
RN: 39227-53-7 **MP** (°C)**:** 98
MW: 218.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.220E-07	1.360E-04	5	S352	2 2 0 2 2	
1.066E-06	2.330E-04	15	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
3.316E-06	7.250E-04	35	S352	2 2 0 2 2	
5.671E-06	1.240E-03	45	S352	2 2 0 2 2	

2681. $C_{12}H_7ClO_2$
2-Chlorodibenzo-*p*-dioxin
2-Monochlorodibenzo-*p*-dioxin
PCDD 2
RN: 39227-54-8 **MP** (°C)**:** 89
MW: 218.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-07	1.334E-04	3.90	D330	2 2 1 2 2	
2.904E-07	6.350E-05	5	S352	2 2 0 2 2	
6.266E-07	1.370E-04	15	S352	2 2 0 2 2	
1.363E-06	2.980E-04	25	S352	2 2 0 2 2	average of 2
1.271E-06	2.780E-04	25	S352	2 2 0 2 2	
1.460E-06	3.192E-04	25.0	D330	2 2 1 2 2	
2.987E-06	6.530E-04	35	S352	2 2 0 2 2	
3.430E-06	7.499E-04	39.0	D330	2 2 1 2 2	
5.072E-06	1.109E-03	45	S352	2 2 0 2 2	

2682. $C_{12}H_7Cl_2NO_3$
Nitrofen
2,4-Dichlorophenyl-4-nitrophenyl ether
RN: 1836-75-5 **MP** (°C)**:** 70.5
MW: 284.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.520E-06	1.000E-03	22	M061	1 0 0 0 0	
3.344E-05	9.500E-03	22	M161	1 0 0 0 0	
3.520E-06	1.000E-03	ns	B100	0 0 0 0 0	
2.144E-06	6.090E-04	ns	H322	0 0 0 0 0	

2683. $C_{12}H_7Cl_3$
2,2′,4-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,4-trichloro-
RN: 37680-66-3 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.006E-06	2.592E-04	20	M336	2 0 2 2 2	

2684. $C_{12}H_7Cl_3$
2,2′,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,6-trichloro-
RN: 38444-73-4 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-06	4.483E-04	20	M336	2 0 2 2 2	

2685. $C_{12}H_7Cl_3$
2,3′,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,3′,6-trichloro-
RN: 38444-76-7 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.498E-07	3.858E-05	20	M336	2 0 2 2 2	

2686. $C_{12}H_7Cl_3$
2,4,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,4,5-trichloro-
RN: 15862-07-4 **MP** (°C)**:** 77
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-07	8.500E-05	23	W024	0 0 0 0 0	
5.436E-07	1.400E-04	25	B319	2 0 1 2 1	
5.514E-07	1.420E-04	25	H341	1 0 0 0 2	
6.320E-07	1.628E-04	25	M342	1 0 1 1 2	
3.572E-07	9.200E-05	25	W025	1 0 2 2 1	
6.320E-07	1.628E-04	ns	M308	0 0 1 1 2	

2687. $C_{12}H_7Cl_3$
2,3,4′-Trichlorobiphenyl
1,1′-Biphenyl, 2,3,4′-trichloro-
RN: 38444-85-8 **MP** (°C)**:** 69
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-07	1.417E-04	20	M336	2 0 2 2 2	

2688. $C_{12}H_7Cl_3$
2,3,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,3,6-trichloro-
RN: 55702-45-9 **MP** (°C)**:** 49
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.126E-07	1.320E-04	20	M336	2 0 2 2 2	

2689. $C_{12}H_7Cl_3$
2,2′,3-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,3-trichloro-
RN: 38444-78-9 **MP** (°C)**:** 28.1
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-06	2.930E-04	20	M336	2 0 2 2 2	

2690. $C_{12}H_7Cl_3$
2,2′,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,5-trichloro-
PCB 18
RN: 37680-65-2 **MP** (°C)**:** 44
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-06	2.986E-04	20	M336	2 0 2 2 2	
1.980E-06	5.099E-04	25	D306	2 1 2 2 2	
2.485E-06	6.400E-04	25	W025	1 0 2 2 2	
4.271E-07	1.100E-04	ns	B301	0 2 1 1 2	
9.629E-07	2.480E-04	ns	H058	0 1 2 1 2	
6.212E-08	1.600E-05	ns	M118	0 1 1 1 1	

2691. $C_{12}H_7Cl_3$
3,4,4′-Trichlorobiphenyl
3,4,4′-Trichlorbiphenyl
RN: 38444-90-5 **MP** (°C)**:** 88
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.791E-07	7.189E-05	20	M336	2 0 2 2 2	
3.106E-07	8.000E-05	23	W024	0 0 0 0 0	
5.902E-08	1.520E-05	25	W025	1 0 2 2 2	

2692. $C_{12}H_7Cl_3$
2,4′,5-Trichlorobiphenyl
2,5,4′-Trichlorobiphenyl
PCB 31
RN: 16606-02-3 **MP** (°C)**:** 67
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
3.494E-07	9.000E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	22.5	G301	0 0 0 0 0	
2.912E-07	7.500E-05	ns	B301	0 2 1 1 1	

2693. $C_{12}H_7Cl_3$
2,4,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,4,6-trichloro-
RN: 35693-92-6 **MP** (°C)**:** 62.5
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	8.036E-05	4.0	D330	2 2 1 2 2	
9.800E-07	2.524E-04	25	D306	2 1 2 2 2	
9.333E-07	2.404E-04	25	L322	1 1 2 2 2	
8.760E-07	2.256E-04	25	M342	1 0 1 1 2	
7.250E-07	1.867E-04	25.0	D330	2 2 1 2 2	
1.690E-06	4.353E-04	40.0	D330	2 2 1 2 2	
8.760E-07	2.256E-04	ns	M308	0 0 1 1 2	

2694. $C_{12}H_7Cl_3$
2,4,4′-Trichlorobiphenyl
2,4,4′-PCB
RN: 7012-37-5 **MP** (°C)**:** 57
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.465E-07	1.150E-04	20	C302	1 1 2 2 2	
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
2.601E-07	6.700E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	24	C311	0 0 0 0 0	EFG
4.504E-07	1.160E-04	25	C313	0 0 0 0 0	
4.530E-07	1.167E-04	25	D306	2 1 2 2 2	
1.010E-06	2.600E-04	25	W025	1 0 2 2 2	

2695. $C_{12}H_7Cl_3$
Aroclor 1242
Arochlor 1242
RN: 53469-21-9 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.377E-07	1.900E-04	4	M336	2 0 2 2 2	
5.160E-07	1.329E-04	11.5	D085	0 0 0 0 0	
1.076E-06	2.770E-04	20	M336	2 0 2 2 2	
7.766E-07	2.000E-04	20	N326	1 0 0 0 2	
1.747E-07	4.500E-05	ns	L106	0 0 2 1 1	
7.766E-07	2.000E-04	ns	M184	0 0 0 0 0	

2696. $C_{12}H_7Cl_3$
2′,3,4-Trichlorobiphenyl
1,1′-Biphenyl, 2′,3,4-trichloro-
RN: 38444-86-9 **MP** (°C)**:** 60.0
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.147E-07	1.326E-04	20	M336	2 0 2 2 2	
1.165E-07	3.000E-05	23	W024	0 0 0 0 0	

2697. $C_{12}H_7Cl_3$
2,3′,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,3′,5-trichloro-
RN: 38444-81-4 **MP** (°C)**:** 40
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E-07	1.384E-04	20	M336	2 0 2 2 2	
9.810E-07	2.527E-04	25	D306	2 1 2 2 2	

2698. $C_{12}H_7Cl_3$
Trichlorobiphenyl
Apirolio 1431C
Pyranol 1499
Pyralene 3011
RN: 25323-68-6 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.620E-07	1.190E-04	11.5	D085	0 0 0 0 0	mixed isomers

2699. $C_{12}H_7Cl_3O_2$
Triclosan
5-Chloro-2-(2,4-dichlorophenoxy)-phenol
RN: 3380-34-5 **MP** (°C)**:** 55.2
MW: 289.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.454E-05	1.000E-02	20	A067	1 0 0 0 0	
		amb	L434	0 0 0 0 0	
3.467E-05	1.004E-02	ns	R427	0 0 0 0 0	

2700. $C_{12}H_7NO_2$
1,8-Naphthalimide
1,8-Naphthalenedicarboximide
Naphthalimide
1,8-Naphthalenedicarboxylic acid imide
1H-Benz[de]isoquinoline-1,3(2H)-dione
RN: 81-83-4 **MP** (°C)**:** 292-300
MW: 197.20 **BP** (°C)**:** 428.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	5.916E-03	23	B410	2 1 2 2 2	

2701. $C_{12}H_7N_3O_2$
5-Nitro-1,10-phenanthroline
5-Nitro-*o*-phenanthroline
RN: 4199-88-6 **MP** (°C)**:**
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.210E-04	2.725E-02	25.04	B094	1 2 1 2 2	

2702. $C_{12}H_7N_5O_8$
2,4,5,6-Tetranitrodiphenylamine
RN: **MP** (°C)**:**
MW: 349.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-04	8.199E-02	13.5	D070	1 2 0 0 1	
2.949E-04	1.030E-01	50	D070	1 2 0 0 2	
5.783E-04	2.020E-01	100	D070	1 2 0 0 2	

2703. $C_{12}H_7N_5O_8$
2,4,2′,4′-Tetranitrodiphenylamine
2,4,2′,4-Tetranitro-diphenylamin
RN: 2908-76-1 **MP** (°C)**:**
MW: 349.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.727E-04	2.000E-01	100	F300	1 0 0 0 2	

2704. $C_{12}H_8$
Acenaphthylene
1,2-Dehydroacenaphthalene
Acenaphthalene
RN: 208-96-8 **MP** (°C)**:** 93.5–94.5
MW: 152.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-05	3.930E-03	25	L332	1 1 1 1 2	

2705. $C_{12}H_8Br_2$
4,4′-Dibromobiphenyl
p,p′-Dibromobiphenyl
RN: 92-86-4 **MP** (°C)**:** 170
MW: 312.02 **BP** (°C)**:** 357

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-02	5.743E+00	26.5	G312	0 0 0 0 0	

2706. $C_{12}H_8Br_2O$
4,4′-Dibromodiphenylether
bis-p-Bromophenyl ether
Dibromodiphenyl ether, *p,p′*-
RN: 2050-47-7 **MP** (°C)**:** 59 C
MW: 328.01 **BP** (°C)**:** 357 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.878E-07	9.440E-05	10	K431	0 0 0 0 0	
6.585E-07	2.160E-04	25	K431	0 0 0 0 0	
1.171E-06	3.840E-04	35	K431	0 0 0 0 0	

2707. $C_{12}H_8Cl_2$
2,5-Dichlorobiphenyl
1,1′-Biphenyl, 2,5-dichloro-
RN: 34883-39-1 **MP** (°C)**:** 23
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.454E-06	1.440E-03	23	W024	0 0 0 0 0	
5.000E-06	1.116E-03	25	D306	2 1 2 2 2	
8.700E-06	1.941E-03	25	M342	1 0 1 1 1	
2.600E-06	5.800E-04	25	W025	1 0 2 2 2	
8.516E-07	1.900E-04	ns	B301	0 2 1 1 2	
2.680E-05	5.979E-03	ns	M308	0 0 1 1 2	

2708. $C_{12}H_8Cl_2$
2,4-Dichlorobiphenyl
1,1′-Biphenyl, 2,4-dichloro-
RN: 33284-50-3 **MP** (°C)**:** 25.0
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.747E-06	6.129E-04	20	M336	2 0 2 2 2	
3.138E-07	7.000E-05	23	W024	0 0 0 0 0	*sic*
5.065E-06	1.130E-03	25	B319	2 0 1 2 2	
5.065E-06	1.130E-03	25	B350	1 0 0 0 2	
5.150E-06	1.149E-03	25	D306	2 1 2 2 2	

2709. $C_{12}H_8Cl_2$
2,4′-Dichlorobiphenyl
2,4′-PCB
RN: 34883-43-7 **MP** (°C)**:** 43
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-06	6.370E-04	20	C302	1 1 2 2 2	
2.413E-06	5.383E-04	20	M336	2 0 2 2 2	
2.241E-06	5.000E-04	24	H100	2 0 2 2 0	
2.779E-06	6.200E-04	25	W025	1 0 2 2 2	
2.855E-06	6.370E-04	ns	H058	0 1 2 1 2	

2710. $C_{12}H_8Cl_2$
2,3′-Dichlorobiphenyl
1,1′-Biphenyl, 2,3′-dichloro-
RN: 25569-80-6 **MP** (°C)**:**
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-06	5.798E-04	20	M336	2 0 2 2 2	

2711. $C_{12}H_8Cl_2$
2,6-Dichlorobiphenyl
1,1′-Biphenyl, 2,6-dichloro-
PCB 10
RN: 33146-45-1 **MP** (°C)**:** 35
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-06	5.400E-04	22	O311	2 2 1 2 2	
1.080E-05	2.410E-03	25	D306	2 1 2 2 2	
6.230E-06	1.390E-03	25	M342	1 0 1 1 2	
6.230E-06	1.390E-03	ns	M308	0 0 1 1 2	

2712. $C_{12}H_8Cl_2$
2,2′-Dichlorobiphenyl
2,2′-PCB
RN: 13029-08-8 **MP** (°C)**:** 61
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.214E-06	7.170E-04	20	C302	1 1 2 2 2	
5.038E-06	1.124E-03	20	M336	2 0 2 2 2	
3.541E-06	7.900E-04	22.5	G301	0 0 0 0 0	

(*continued*)

2712. $C_{12}H_8Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.275E-06	1.400E-03	23	W024	0 0 0 0 0	
4.034E-06	9.000E-04	24	H100	2 0 2 2 0	
5.410E-06	1.207E-03	25	D306	2 1 2 2 2	
3.541E-06	7.900E-04	25	W025	1 0 2 2 2	

2713. $C_{12}H_8Cl_2$

3,4-Dichlorobiphenyl
1,1′-Biphenyl, 3,4-dichloro-
RN: 2974-92-7 **MP** (°C)**:** 49.5
MW: 223.10 **BP** (°C)**:** 197.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.550E-08	7.920E-06	25	D306	2 1 2 2 2	
4.074E-07	9.089E-05	ns	R424	0 0 0 0 0	

2714. $C_{12}H_8Cl_2$

4,4′-Dichlorobiphenyl
4,4′-PCB
Dichlorobiphenyl
RN: 2050-68-2 **MP** (°C)**:** 149
MW: 223.10 **BP** (°C)**:** 317

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.488E-06	3.320E-04	11.5	D085	0 0 0 0 0	mixed isomers
2.779E-07	6.200E-05	20	C053	0 0 0 0 0	
2.779E-07	6.200E-05	20	F071	1 1 1 1 1	
2.779E-07	6.200E-05	20	M344	1 0 0 0 1	
2.689E-07	6.000E-05	24	H100	2 0 2 2 0	
2.376E-07	5.300E-05	25	B319	2 0 1 2 2	average of 2
2.062E-07	4.600E-05	25	B350	1 0 0 0 1	
1.630E-07	3.637E-05	25	D306	2 1 2 2 2	
2.913E-07	6.500E-05	25	H341	1 0 0 0 1	
2.510E-07	5.600E-05	25	W025	1 0 2 2 1	

2715. $C_{12}H_8Cl_2$

3,3′-Dichlorobiphenyl
1,1′-Biphenyl, 3,3′-dichloro-
RN: 2050-67-1 **MP** (°C)**:** 29
MW: 223.10 **BP** (°C)**:** 323.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-06	3.547E-04	25	D306	2 1 2 2 2	

2716. $C_{12}H_8Cl_2O_2S$

bis(4-Chlorophenyl) sulfone
4,4′-Dichlorodiphenyl sulfone
1,1′-Sulfonylbis(4-chlorobenzene)
p-Chlorophenyl sulfone

RN: 80-07-9 **MP** (°C)**:** 149 C
MW: 287.17 **BP** (°C)**:** 397 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-07	5.000E-05	22	J420	0 0 0 0 0	pH 6.5

2717. $C_{12}H_8Cl_6$

Aldrin
1,2,3,4,10,10-Hexachloro-1,4,4α,5,8,8α-hexahydro-1,4:5,8-dimethanonaphthalene
Aldrite
Seedrin
Aldrosol
HHDN

RN: 309-00-2 **MP** (°C)**:** 104.3
MW: 364.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.877E-07	1.050E-04	15	B083	2 2 1 2 2	particle size 5 µm
7.413E-08	2.705E-05	20	B179	0 0 0 0 0	
4.659E-08	1.700E-05	22.5	G301	0 0 0 0 0	
4.898E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.933E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 µm
5.481E-07	2.000E-04	25	M130	1 0 0 0 0	
4.659E-08	1.700E-05	25	W025	1 0 2 2 2	
7.399E-08	2.700E-05	26.5	P027	1 1 2 2 1	
5.481E-07	2.000E-04	26.70	L095	2 2 1 1 2	
7.399E-08	2.700E-05	27	M161	0 0 0 0 1	
9.591E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.644E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 µm
7.399E-08	2.700E-05	ns	I308	0 0 0 0 0	
3.562E-08	1.300E-05	ns	K138	0 0 0 0 2	
1.096E-07	4.000E-05	ns	M110	0 0 0 0 0	EFG

2718. $C_{12}H_8Cl_6O$

Endrin
1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4α,5,6,7,8,8α-octahydro-1,4-*endo*-*endo*-5,8-dimethanonaphthalene
Mendrin
Nendrin

RN: 72-20-8 **MP** (°C)**:** 228.0
MW: 380.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.413E-07	1.300E-04	15	B083	2 2 1 2 2	particle size 5 µm
6.607E-07	2.517E-04	24.99	K436	0 0 0 0 0	
6.563E-07	2.500E-04	25	B083	2 2 1 2 2	particle size 5 µm
6.826E-07	2.600E-04	25	W025	1 0 2 2 2	
1.103E-06	4.200E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.641E-06	6.250E-04	45	B083	2 2 1 2 2	particle size 5 µm
6.301E-08	2.400E-05	ns	K138	0 0 0 0 2	
1.050E-06	4.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
6.563E-07	2.500E-04	ns	V414	0 0 0 0 0	

2719. $C_{12}H_8Cl_6O$

Dieldrin
3,4,5,6,9,9-Hexachloro-1α,2,2α,3,6,6α,7,7α-octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene
Alvit
Quintox
Oxralox

RN: 60-57-1 **MP** (°C)**:** 175.5
MW: 380.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-07	7.999E-05	10	B324	0 0 0 0 0	
2.100E-07	8.000E-05	10	B324	0 0 0 0 0	
2.363E-07	9.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
4.898E-07	1.866E-04	20	B179	0 0 0 0 0	
3.675E-07	1.400E-04	20	B324	0 0 0 0 0	
3.676E-07	1.400E-04	20	B324	0 0 0 0 0	
1.229E-06	4.680E-04	22	K137	1 1 2 1 0	
5.129E-07	1.954E-04	24.99	K436	0 0 0 0 0	
5.119E-07	1.950E-04	25	B083	2 2 1 2 2	particle size 5 µm
4.883E-07	1.860E-04	25	I308	0 0 0 0 0	
6.563E-07	2.500E-04	25	M130	1 0 0 0 1	
5.251E-07	2.000E-04	25	W025	1 0 2 2 2	
1.313E-07	5.000E-05	26	M061	1 0 0 0 0	
4.883E-07	1.860E-04	26.5	P027	1 1 2 2 2	
5.251E-07	2.000E-04	27	B161	2 1 2 2 0	EFG
4.883E-07	1.860E-04	27	M161	0 0 0 0 2	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	

(*continued*)

2719. $C_{12}H_8Cl_6O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-06	4.000E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.313E-06	5.000E-04	40	B161	2 1 2 2 0	EFG
1.706E-06	6.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
2.363E-06	9.000E-04	50	B161	2 1 2 2 0	EFG
3.544E-06	1.350E-03	60	B161	2 1 2 2 0	EFG
6.511E-06	2.480E-03	70	B161	2 1 2 2 0	EFG
6.563E-07	2.500E-04	ns	H322	0 0 0 0 0	
5.776E-08	2.200E-05	ns	K138	0 0 0 0 2	
7.876E-07	3.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
5.119E-07	1.950E-04	ns	V414	0 0 0 0 0	

2720. $C_{12}H_8N_2$

p-Phenanthroline
p-Phenanthrolin
RN: 230-07-9 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.442E+00	ns	K114	0 0 0 0 0	

2721. $C_{12}H_8N_2$

Phenazine
Dibenzopyrazine
RN: 92-82-0 **MP** (°C)**:** 175.5
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	2.523E-02	25	K009	1 2 1 1 0	EFG

2722. $C_{12}H_8N_2$

o-Phenanthroline
1,10-Phenanthroline
o-Phenanthrolin
RN: 66-71-7 **MP** (°C)**:** 115
MW: 180.21 **BP** (°C)**:** >300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-02	3.340E+00	24.99	B444	0 0 0 0 0	
1.526E-02	2.750E+00	25	M155	1 0 1 1 0	EFG
1.490E-02	2.685E+00	25.04	B094	1 2 1 2 2	
1.850E-02	3.334E+00	31	B094	1 2 1 2 2	

(*continued*)

2722. $C_{12}H_8N_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-02	3.766E+00	35	B094	1 2 1 2 2	
2.550E-02	4.595E+00	40.04	B094	1 2 1 2 2	
2.880E-02	5.190E+00	45.44	B094	1 2 1 2 2	
3.410E-02	6.145E+00	50.04	B094	1 2 1 2 2	

2723. $C_{12}H_8N_2$
m-Phenanthroline
m-Phenanthrolin
RN: 230-46-6 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	7.208E-01	ns	K114	0 0 0 0 0	

2724. $C_{12}H_8N_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-benzoyl-1,5-dihydro-
RN: 96448-63-4 **MP** (°C)**:**
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.828E-05	1.400E-02	22	B428	1 2 1 2 1	

2725. $C_{12}H_8N_4O_6$
Picrylaniline
2,4,6-Trinitrodiphenyllamine
RN: 2919-12-2 **MP** (°C)**:**
MW: 304.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-05	1.791E-02	25	B335	1 2 0 0 1	

2726. $C_{12}H_8O$
Dibenzofuran
Diphenylene oxide
DBF
RN: 132-64-9 **MP** (°C)**:** 83
MW: 168.20 **BP** (°C)**:** 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.820E-06	1.652E-03	4.0	D330	2 2 1 2 2	
5.960E-05	1.002E-02	25	B173	2 0 2 2 2	

(*continued*)

2726. $C_{12}H_8O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.112E-03	25	L301	1 1 2 2 2	
2.592E-05	4.360E-03	25	O406	0 0 0 0 0	
2.812E-05	4.730E-03	25	O406	0 0 0 0 0	
2.510E-05	4.222E-03	25.0	D330	2 2 1 2 2	
4.140E-05	6.963E-03	39.8	D330	2 2 1 2 2	

2727. $C_{12}H_8O_2$

Dibenzo-*p*-dioxin
Dibenzo[1,4]dioxin
Oxanthrene
Phenodioxin

RN: 262-12-4 **MP** (°C)**:** 119
MW: 184.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-06	2.118E-04	4.10	D330	2 2 1 2 2	
1.113E-06	2.050E-04	5	S352	2 2 0 2 2	
2.497E-06	4.600E-04	15	S352	2 2 0 2 2	
7.601E-06	1.400E-03	25	O406	0 0 0 0 0	
6.841E-06	1.260E-03	25	O406	0 0 0 0 0	
4.729E-06	8.710E-04	25	S352	2 2 0 2 2	average of 2
4.571E-06	8.420E-04	25	S352	2 2 0 2 2	
4.890E-06	9.007E-04	25.0	D330	2 2 1 2 2	
9.566E-06	1.762E-03	35	S352	2 2 0 2 2	
1.300E-05	2.395E-03	40.0	D330	2 2 1 2 2	
1.771E-05	3.262E-03	45	S352	2 2 0 2 2	

2728. $C_{12}H_8O_4$

Methoxsalen
Ammoidin
8-Methoxy-2′,3′,6,7-furocoumarin
Methoxalen
8-Methoxyfuranocoumarin
Oxypsoralen

RN: 298-81-7 **MP** (°C)**:** 148
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	4.756E-02	30	E012	1 2 1 1 0	

2729. $C_{12}H_8S$

Dibenzothiophene
Diphenylene sulfide

RN: 132-65-0 **MP** (°C)**:** 97
MW: 184.26 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.978E-06	1.470E-03	24	H106	1 0 2 2 2	
7.978E-06	1.470E-03	24	M303	1 0 1 1 2	
2.871E-06	5.291E-04	25	L301	1 1 2 2 2	
7.978E-06	1.470E-03	ns	H107	0 0 0 0 2	

2730. $C_{12}H_9Br$

4-Bromobiphenyl
1,1′-Biphenyl, 4-bromo-
Bromodiphenyl

RN: 92-66-0 **MP** (°C)**:** 91.5
MW: 233.11 **BP** (°C)**:** 310.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-06	2.354E-04	4.0	D330	2 2 1 2 2	
2.800E-06	6.527E-04	25.0	D330	2 2 1 2 2	
3.740E-06	8.718E-04	40.0	D330	2 2 1 2 2	

2731. $C_{12}H_9Cl$

2-Chlorobiphenyl
2-PCB

RN: 2051-60-7 **MP** (°C)**:** 32
MW: 188.66 **BP** (°C)**:** 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-05	3.760E-03	20	C302	1 1 2 2 2	
3.074E-05	5.800E-03	23	W024	0 0 0 0 0	
4.771E-06	9.000E-04	24	H100	2 0 2 2 0	
4.134E-05	7.800E-03	25	B351	1 0 0 1 1	
2.680E-05	5.056E-03	25	M342	1 0 1 1 2	
2.189E-05	4.130E-03	25	W025	1 0 2 2 2	
2.680E-05	5.056E-03	ns	M308	0 0 1 1 2	

2732. $C_{12}H_9Cl$
4-Chlorobiphenyl
1-Chloro-4-phenyl benzene
4-Monochloro-biphenyl
RN: 2051-62-9 **MP** (°C)**:** 77
MW: 188.66 **BP** (°C)**:** 291

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.202E-06	1.170E-03	23	W024	0 0 0 0 0	
2.120E-06	4.000E-04	24	H100	2 0 2 2 0	
7.103E-06	1.340E-03	25	B319	2 0 1 2 2	average of 2
6.891E-06	1.300E-03	25	B350	1 0 0 0 2	
6.361E-06	1.200E-03	25	B351	1 0 0 1 1	
6.361E-06	1.200E-03	25	H341	1 0 0 0 2	
7.087E-06	1.337E-03	25	L322	1 1 2 2 2	average of 2
7.079E-06	1.336E-03	25	L322	1 1 2 2 2	average of 2
4.771E-06	9.000E-04	25	W025	1 0 2 2 2	

2733. $C_{12}H_9Cl$
3-Chlorobiphenyl
3-Chlorbiphenyl
RN: 2051-61-8 **MP** (°C)**:** 16
MW: 188.66 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.908E-05	3.600E-03	23	W024	0 0 0 0 0	
9.806E-06	1.850E-03	23	W024	0 0 0 0 0	
1.924E-05	3.630E-03	25	B319	2 0 1 2 2	
6.891E-06	1.300E-03	25	W025	1 0 2 2 2	

2734. $C_{12}H_9Cl$
Aroclor 1221
Arochlor 1221
RN: 11104-28-2 **MP** (°C)**:**
MW: 188.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.06E-06	>2.00E-04	ns	M184	0 0 0 0 0	

2735. $C_{12}H_9ClF_3N_3O$

Norflurazon
4-Chloro-5-(methylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3(2H)-pyridazinone
Zorial
RN: 27314-13-2 **MP** (°C)**:** 177
MW: 303.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.220E-05	2.800E-02	23	M161	1 0 0 0 1	
9.220E-05	2.800E-02	24	C105	2 1 2 2 2	
9.220E-05	2.800E-02	25	B310	1 1 0 0 1	

2736. $C_{12}H_9ClN_2$

4-Chloroazobenzene
Diazene, (4-chlorophenyl)phenyl-, (E)-
RN: 4340-77-6 **MP** (°C)**:** 88
MW: 216.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	4.333E-04	25	B333	0 0 0 0 0	

2737. $C_{12}H_9ClO$

4-Chlorophenyl phenyl ether
1-Chloro-4-phenoxybenzene
p-Chlorodiphenyl oxide
RN: 7005-72-3 **MP** (°C)**:**
MW: 204.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.612E-05	3.300E-03	25	B131	1 0 0 0 1	

2738. $C_{12}H_9Cl_2NO_2S$

N-(2,3-Chlorophenyl)-benzene-sulfonamide
RN: **MP** (°C)**:**
MW: 302.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-05	5.809E-03	20	P433	0 0 0 0 0	
2.256E-05	6.816E-03	25	P433	0 0 0 0 0	
2.717E-05	8.209E-03	30	P433	0 0 0 0 0	
3.511E-05	1.061E-02	37	P433	0 0 0 0 0	
4.300E-05	1.299E-02	42	P433	0 0 0 0 0	

2739. $C_{12}H_9Cl_2NO_3$
Vinclozolin
3-(3,5-Dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione
Ornalin
Vinclozalin
Ronilan
RN: 50471-44-8 **MP** (°C)**:** 108
MW: 286.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.495E-03	1.000E+00	20	M161	1 0 0 0 0	
9.120E-06	2.609E-03	ns	R427	0 0 0 0 0	

2740. $C_{12}H_9Cl_3NO_2S$
Reserptyl
4′-[Chlorophenyl}-3,4-dichlorophenylbenzene-sulphonamide
RN: **MP** (°C)**:** 127–129
MW: 337.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-04	3.600E-02	25	L014	1 0 1 1 1	

2741. $C_{12}H_9FN_2O_4$
1-Benzyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, phenylmethyl ester
RN: 66999-98-2 **MP** (°C)**:**
MW: 264.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-04	8.000E-02	22	B332	1 1 0 0 1	pH 4.0

2742. $C_{12}H_9N$
Carbazole
9-Azafluorene
Dibenzo[b,d]pyrrole
Diphenylenimine
9H-Carbazole
Dibenzopyrrole
RN: 86-74-8 **MP** (°C)**:** 245
MW: 167.21 **BP** (°C)**:** 355

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.177E-06	1.200E-03	20	H300	1 1 2 2 1	
5.427E-06	9.075E-04	25	L301	1 1 2 2 2	

2743. $C_{12}H_9NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-methyl-
RN: 74103-11-0 **MP** (°C)**:**
MW: 215.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-07	7.000E-05	25	P089	0 0 0 0 0	
4.321E-07	9.300E-05	37	P089	0 0 0 0 0	
5.529E-07	1.190E-04	51	P089	0 0 0 0 0	

2744. $C_{12}H_9NS$
Phenothiazine
Dibenzo-1,4-thiazine
Thiodiphenylamine
RN: 92-84-2 **MP** (°C)**:** 185.1
MW: 199.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.196E-03	20	M177	2 2 2 2 0	EFG
8.000E-06	1.594E-03	25	M177	2 2 2 2 0	EFG
1.000E-05	1.993E-03	30	M177	2 2 2 2 0	EFG

2745. $C_{12}H_9N_3O_2$
4-Nitroazobenzene
Diazene, (*p*-nitrophenyl)phenyl-, (E)-
RN: 2491-52-3 **MP** (°C)**:**
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	6.362E-04	25	B333	0 0 0 0 0	

2746. $C_{12}H_9N_3O_3$
Dis. A. 3
4-[(4-Nitrophenyl)azo]phenol
p-Nitrophenylazophenol
p-Hydroxy-*p′*-nitroazobenzene
RN: 1435-60-5 **MP** (°C)**:** 216
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.892E-03	25	B333	0 0 0 0 0	

2747. $C_{12}H_9N_3O_4$
2,4-Dinitrodiphenylamine
2,4-Dinitrodiphenylamin
C.I. Disperse yellow 14
RN: 961-68-2 **MP** (°C)**:** 160
MW: 259.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.466E-04	3.800E-02	15	D070	1 2 0 0 1	
1.543E-04	4.000E-02	15	F300	1 0 0 0 0	
5.100E-06	1.322E-03	25	B333	0 0 0 0 0	*sic*
3.240E-04	8.399E-02	50	D070	1 2 0 0 1	
5.516E-04	1.430E-01	100	D070	1 2 0 0 2	

2748. $C_{12}H_9N_3O_5$
C.I. Disperse yellow 1
C.I. Disperse yellow 1
p-(2,4-Dinitroanilino)
2,4-Dinitro-4′-hydroxydiphenylamine
4-Hydroxy-2′,4′-dinitrodiphenylamine
RN: 119-15-3 **MP** (°C)**:** 194
MW: 275.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-06	2.477E-03	25	B333	0 0 0 0 0	
6.195E-05	1.705E-02	60	P313	0 0 0 0 0	average of 2
1.546E-04	4.255E-02	70	P313	0 0 0 0 0	average of 2
2.954E-04	8.130E-02	80	P313	0 0 0 0 0	average of 2
5.559E-04	1.530E-01	90	P313	0 0 0 0 0	average of 2
1.163E-03	3.200E-01	100	P313	0 0 0 0 0	

2749. $C_{12}H_9N_5O_3$
1-Nicotinoyloxymethyl allopurinol
3-Pyridinecarboxylic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98846-66-3 **MP** (°C)**:** 242–243
MW: 271.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.429E-04	9.300E-02	22	B322	0 0 0 0 0	

2750. $C_{12}H_{10}$

Diphenyl
Biphenyl
Phenylbenzene
1,1′-Biphenyl
Lemonene

RN: 92-52-4 **MP** (°C)**:** 69.1
MW: 154.21 **BP** (°C)**:** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E-05	2.650E-03	–.7	N053	1 0 0 1 0	EFG
1.973E-05	3.042E-03	4.62	N053	1 0 0 1 0	EFG
2.670E-05	4.118E-03	10	J302	2 1 2 2 2	
2.372E-05	3.658E-03	10.13	N053	1 0 0 1 0	EFG
2.918E-05	4.500E-03	14.20	N053	1 0 0 1 0	EFG
3.800E-05	5.860E-03	20	H306	1 0 1 2 1	
4.182E-05	6.450E-03	20	T301	1 2 2 2 2	
3.590E-05	5.536E-03	20.10	N053	1 0 0 1 0	EFG
4.100E-05	6.323E-03	21	A057	2 1 2 2 1	
4.533E-05	6.990E-03	22	C413	2 0 2 2 1	
4.850E-05	7.480E-03	22.5	G301	0 0 0 0 0	
1.187E-04	1.830E-02	23.5	S171	2 1 2 2 2	
2.983E-05	4.600E-03	24	H100	2 0 2 2 1	
5.512E-05	8.500E-03	24	H116	2 1 0 0 2	
4.708E-05	7.260E-03	24.60	W003	2 2 2 2 2	average of 3
3.852E-05	5.940E-03	25	A001	1 0 2 2 2	
4.570E-05	7.048E-03	25	A325	2 1 2 2 2	
4.850E-05	7.480E-03	25	B003	2 2 2 2 2	
3.910E-05	6.030E-03	25	B173	2 0 2 2 2	
4.799E-05	7.400E-03	25	B319	2 0 1 2 1	average of 2
4.409E-05	6.800E-03	25	B351	1 0 0 1 1	
4.831E-05	7.450E-03	25	E004	2 1 2 2 2	
4.850E-05	7.479E-03	25	J302	2 1 2 2 2	
4.863E-05	7.500E-03	25	M040	1 0 0 1 1	
4.539E-05	7.000E-03	25	M064	1 1 2 2 1	
4.850E-05	7.480E-03	25	M130	1 0 0 0 2	
4.350E-05	6.708E-03	25	M342	1 0 1 1 2	
4.540E-05	7.001E-03	25	M342	1 0 1 1 2	
4.234E-04	6.530E-02	25	S005	2 2 2 2 2	
4.910E-05	7.572E-03	25.04	V013	2 2 2 2 2	
4.416E-05	6.811E-03	25.35	N053	1 0 0 1 0	EFG
5.689E-05	8.774E-03	28.95	N053	1 0 0 1 0	EFG
5.700E-05	8.790E-03	29.90	W003	2 2 2 2 2	average of 3
5.525E-05	8.520E-03	30.30	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	38.40	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	40.10	W003	2 2 2 2 2	average of 3
1.219E-04	1.880E-02	47.50	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.10	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.20	W003	2 2 2 2 2	average of 2
1.855E-04	2.860E-02	54.70	W003	2 2 2 2 2	average of 3

(*continued*)

2750. $C_{12}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-04	3.620E-02	59.20	W003	2 2 2 2 2	average of 3
2.620E-04	4.040E-02	60.50	W003	2 2 2 2 2	
2.918E-04	4.500E-02	64.50	W003	2 2 2 2 2	average of 3
4.539E-05	7.000E-03	ns	H123	0 0 0 0 0	
4.350E-05	6.708E-03	ns	M308	0 0 1 1 2	
4.539E-05	7.000E-03	ns	M344	0 0 0 0 1	

2751. $C_{12}H_{10}$

Acenaphthene
1,2-Dihydroacenaphthene
1,8-Ethylenenaphthalene
peri-Ethylenenaphthalene

RN: 83-32-9 **MP** (°C)**:** 95
MW: 154.21 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.315E-05	3.570E-03	22.20	W003	2 2 2 2 2	
4.780E-05	7.371E-03	25	B173	2 0 2 2 2	
2.250E-05	3.470E-03	25	E004	2 1 2 2 2	
2.218E-05	3.420E-03	25	L332	1 1 1 1 2	
2.548E-05	3.930E-03	25	M064	1 1 2 2 2	
2.550E-05	3.932E-03	25	M342	1 0 1 1 2	
8.889E-07	1.371E-04	25	R084	2 2 2 2 1	*sic*
2.330E-05	3.593E-03	25.04	V013	2 2 2 2 2	
3.041E-05	4.690E-03	30.00	W003	2 2 2 2 2	average of 3
3.761E-05	5.800E-03	34.50	W003	2 2 2 2 2	average of 3
4.520E-05	6.970E-03	39.30	W003	2 2 2 2 1	average of 3
6.076E-05	9.370E-03	44.70	W003	2 2 2 2 1	average of 3
8.060E-05	1.243E-02	50.10	W003	2 2 2 2 2	average of 3
1.038E-04	1.600E-02	55.60	W003	2 2 2 2 2	average of 3
1.741E-04	2.685E-02	64.50	W003	2 2 2 2 2	average of 3
1.511E-04	2.330E-02	65.20	W003	2 2 2 2 2	average of 3
2.118E-04	3.267E-02	69.80	W003	2 2 2 2 2	average of 3
2.283E-04	3.520E-02	71.90	W003	2 2 2 2 2	
2.568E-04	3.960E-02	73.40	W003	2 2 2 2 2	average of 2
2.597E-04	4.005E-02	74.70	W003	2 2 2 2 2	average of 2
3.981E-05	6.139E-03	ns	D001	0 0 0 0 2	
2.248E-05	3.467E-03	ns	I332	0 0 0 0 1	
2.000E-05	3.084E-03	ns	L060	0 0 0 0 0	average
2.548E-05	3.930E-03	ns	M344	0 0 0 0 2	
2.344E-05	3.615E-03	ns	R424	0 0 0 0 0	

2752. $C_{12}H_{10}ClN$

4-Amino-4′-chlorodiphenyl
4-Chloro-4′-aminobiphenyl
p-Amino-*p*′-chlorobiphenyl
p′-Chloro-*p*-phenylaniline

RN: 135-68-2 **MP** (°C)**:**
MW: 203.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	4.684E-03	ns	B305	0 2 0 0 1	

2753. $C_{12}H_{10}ClNO_2S$

N-(2-Chlorophenyl)-benzene-sulfonamide

RN: **MP** (°C)**:**
MW: 267.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-05	1.119E-02	20	P433	0 0 0 0 0	
4.800E-05	1.285E-02	25	P433	0 0 0 0 0	
5.239E-05	1.403E-02	30	P433	0 0 0 0 0	
5.667E-05	1.517E-02	37	P433	0 0 0 0 0	
6.444E-05	1.725E-02	42	P433	0 0 0 0 0	

2754. $C_{12}H_{10}ClNO_2S$

N-(4-Chlorophenyl)-benzene-sulfonamide

RN: **MP** (°C)**:**
MW: 267.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.611E-05	2.038E-02	20	P433	0 0 0 0 0	
9.333E-05	2.499E-02	25	P433	0 0 0 0 0	
1.244E-04	3.332E-02	30	P433	0 0 0 0 0	
1.789E-04	4.789E-02	37	P433	0 0 0 0 0	
2.189E-04	5.860E-02	42	P433	0 0 0 0 0	

2755. $C_{12}H_{10}Cl_2N_2$

3,3′-Dichlorobenzidine
3,3′-Dichloro-4,4′-biphenyldiamine
o,*o*′-Dichlorobenzidine
4,4′-Diamino-3,3′-dichlorobiphenyl

RN: 91-94-1 **MP** (°C)**:** 132
MW: 253.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.114E-03	25	B173	2 0 2 2 2	
<3.95E-06	<1.00E-03	30	M311	1 1 2 2 0	

2756. $C_{12}H_{10}N_2$
Harmane
1-Methyl-9H-pyrido[3,4-b]indole
Aribine
RN: 486-84-0 **MP** (°C)**:** 235–238
MW: 182.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.010E+00	1.095E+03	15	B413	1 0 2 2 1	
6.250E+00	1.139E+03	16	B413	1 0 2 2 1	
6.710E+00	1.223E+03	17	B413	1 0 2 2 1	
8.360E+00	1.523E+03	20	B413	1 0 2 2 1	
1.364E+01	2.486E+03	37	B413	1 0 2 2 1	
1.434E+01	2.613E+03	38	B413	1 0 2 2 1	
1.617E+01	2.947E+03	45	B413	1 0 2 2 1	

2757. $C_{12}H_{10}N_2O$
4-Phenylazophenol
4-Hydroxyazobenzene
p-Hydroxyazobenzene
C.I. Solvent yellow 7
RN: 1689-82-3 **MP** (°C)**:** 150
MW: 198.23 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.540E-04	9.000E-02	20	F300	1 0 0 0 1	
1.100E-04	2.180E-02	25	B333	0 0 0 0 0	
1.715E-04	3.400E-02	37	H120	1 1 1 1 1	normal saline
4.036E-03	8.000E-01	100	F300	1 0 0 0 1	

2758. $C_{12}H_{10}N_2O$
Diphenylnitrosamine
Redax
N-Nitroso-*N*-phenylaniline
RN: 86-30-6 **MP** (°C)**:** 67
MW: 198.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-04	3.509E-02	25	B173	2 0 2 2 2	

2759. $C_{12}H_{10}N_2O_2$
2,4-Dihydroxyazobenzene
2,4-Dihydroxy-azobenzol
RN: 2051-85-6 **MP** (°C)**:** 170
MW: 214.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.336E-04	2.000E-01	20	F300	1 0 0 0 0	

2760. $C_{12}H_{10}N_2O_3$
3-Hydroxyazobenzene
3-Hydroxy-azobenzol
RN: 40038-46-8 **MP** (°C)**:**
MW: 230.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.475E-03	8.000E-01	100	F300	1 0 0 0 1	

2761. $C_{12}H_{10}N_4O_2$
C.I. Disperse orange 3
4′-Nitro-4-aminoazobenzene
4-Amino-4′-nitroazobenzene
4-(4-Nitrophenylazo)aniline
RN: 730-40-5 **MP** (°C)**:** 211
MW: 242.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.907E-04	25	B333	0 0 0 0 0	

2762. $C_{12}H_{10}N_4O_4$
C.I. Disperse yellow 9
2,4-Dinitro-4′-aminodiphenylamine
4-Amino-2′,4′-dinitrodiphenylamine
C.I. 10375
RN: 6373-73-5 **MP** (°C)**:** 188
MW: 274.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.645E-03	25	B333	0 0 0 0 0	

2763. $C_{12}H_{10}O$
p-Phenylphenol
p-Hydroxybiphenyl
RN: 92-69-3 **MP** (°C)**:** 164.5
MW: 170.21 **BP** (°C)**:** 306.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	5.617E-02	25	E014	2 2 2 1 2	pH 7.2
5.875E-05	1.000E-02	25	L021	1 0 0 0 0	

2764. $C_{12}H_{10}O$
o-Phenylphenol
2-Phenylphenol
RN: 90-43-7 **MP** (°C)**:** 56.5
MW: 170.21 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.790E-04	1.666E-01	25	L021	1 0 0 0 0	
4.110E-03	6.995E-01	25	M061	0 0 0 0 0	
4.112E-03	7.000E-01	25	M161	1 0 0 0 0	
3.162E-04	5.383E-02	rt	D056	0 1 1 1 0	EFG, pH 6–8, *sic*

2765. $C_{12}H_{10}O$
Phenyl ether
Diphenyl ether
RN: 101-84-8 **MP** (°C)**:** 28
MW: 170.21 **BP** (°C)**:** 259

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.341E-02	3.984E+00	25	B019	1 0 1 2 0	*sic*
1.060E-04	1.804E-02	25	B173	2 0 2 2 2	
1.234E-04	2.100E-02	25	F071	1 1 2 1 1	
1.100E-04	1.872E-02	25.04	V013	2 2 2 2 2	

2766. $C_{12}H_{10}O_2$
1-Naphthaleneacetic acid
NAA
RN: 86-87-3 **MP** (°C)**:** 134
MW: 186.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.040E-03	3.799E-01	17	B200	1 0 0 0 1	
2.255E-03	4.198E-01	20	B200	1 0 0 0 1	
1.179E-02	2.195E+00	20	C092	2 2 0 1 2	
2.228E-03	4.148E-01	25	M061	1 0 0 0 2	average of 2

2767. $C_{12}H_{10}O_2$
2-Hydroxydiphenyl ether
2-Hydroxy-diphenyl-aether
RN: 2417-10-9 **MP** (°C)**:**
MW: 186.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.907E-04	1.100E-01	20	F300	1 0 0 0 1	

2768. $C_{12}H_{10}O_3$
β-Naphthoxyacetic acid
(2-Naphthoxy)acetic acid
Phyomone
BNOA
RN: 120-23-0 **MP** (°C)**:** 155–157
MW: 202.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.330E-04	8.756E-02	25	D088	0 0 0 0 0	
8.100E-04	1.638E-01	35	D088	0 0 0 0 0	
1.100E-05	2.224E-03	45	D088	0 0 0 0 0	

2769. $C_{12}H_{10}O_4$
Quinhydrone
Chinhydron
RN: 106-34-3 **MP** (°C)**:** 171
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.861E-02	4.061E+00	25	B121	1 2 2 1 2	average of 4

2770. $C_{12}H_{11}ClN_2O_5S$
Furosemide
Frusemide
RN: 54-31-9 **MP** (°C)**:** 206
MW: 330.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-05	1.850E-02	20	B405	1 1 1 2 2	
1.814E-05	6.000E-03	22.5	C438	0 0 0 0 0	
1.784E-05	5.900E-03	25	A408	2 0 1 2 0	
2.691E-05	8.900E-03	25	B405	1 1 1 2 2	Buffer pH 2.0
7.559E-05	2.500E-02	25	B405	1 1 1 2 2	
1.875E-05	6.200E-03	25	F415	0 0 0 0 0	Average
2.210E-04	7.310E-02	30	E049	2 0 2 2 2	

(*continued*)

2770. $C_{12}H_{11}ClN_2O_5S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.023E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.778E-05	5.882E-03	ns	R427	0 0 0 0 0	

2771. $C_{12}H_{11}Cl_2NO$

Propyzamide
3,5-Dichloro-*N*-(1,1-dimethyl-2-propynyl)benzamide
Pronamide
Kerb 50W
RH-315

RN: 23950-58-5 **MP** (°C)**:** 155.5
MW: 256.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.856E-05	1.500E-02	25	M161	1 0 0 0 1	

2772. $C_{12}H_{11}I_3N_2O_4$

Iodamide
3-Acetamido-5-acetamidomethyl-2,4,6-triiodobenzoic acid
3-Acetylamino-5-acetylaminomethyl-2,4,6-triiodobenzoic acid
Jodomiron 380
Uromiro
Uromiron

RN: 440-58-4 **MP** (°C)**:**
MW: 627.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.777E-03	3.000E+00	20	F045	1 2 2 2 1	
5.096E-03	3.200E+00	40	F045	1 2 2 2 1	
6.211E-03	3.900E+00	60	F045	1 2 2 2 1	

2773. $C_{12}H_{11}N$

Diphenylamine
4-Aminobiphenyl

RN: 122-39-4 **MP** (°C)**:** 53.5
MW: 169.23 **BP** (°C)**:** 302.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-03	3.079E-01	20	B179	0 0 0 0 0	
3.132E-04	5.300E-02	20	H300	1 2 2 2 1	
3.274E-04	5.540E-02	20	T301	1 2 2 2 2	
2.765E-04	4.680E-02	25	F029	1 0 0 0 2	
3.415E-04	5.780E-02	50	T301	1 2 2 2 2	average of 5
3.557E-04	6.020E-02	80	T301	1 2 2 2 2	average of 5
1.772E-03	2.999E-01	rt	D021	0 0 1 1 0	

2774. $C_{12}H_{11}NO_2$
Fenfuram
2-Methyl-*N*-phenyl-3-furancarboxamide
Pano-ram
RN: 24691-80-3 **MP** (°C)**:** 109.5
MW: 201.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.970E-04	1.000E-01	20	M161	1 0 0 0 0	

2775. $C_{12}H_{11}NO_2$
Carbaryl
1-Naphthyl *N*-methylcarbamate
Devicarb
Hexavin
Karbaspray
Murvin
RN: 63-25-2 **MP** (°C)**:** 142
MW: 201.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	5.453E-02	5	H343	0 0 0 0 0	
3.598E-04	7.239E-02	10	B324	0 0 0 0 0	
3.444E-04	6.930E-02	10	B324	0 0 0 0 0	
3.150E-04	6.339E-02	10	H343	0 0 0 0 0	
3.740E-04	7.526E-02	15	H343	0 0 0 0 0	
1.995E-04	4.015E-02	20	B179	0 0 0 0 0	
5.164E-04	1.039E-01	20	B300	2 1 1 1 2	
4.947E-04	9.955E-02	20	B324	0 0 0 0 0	
5.168E-04	1.040E-01	20	B324	0 0 0 0 0	
2.485E-04	5.000E-02	20	F311	1 2 2 2 1	
4.450E-04	8.955E-02	20	H343	0 0 0 0 0	
1.690E-04	3.400E-02	22	K137	1 1 2 1 0	
1.988E-04	4.000E-02	22.5	G301	0 0 0 0 0	
5.210E-04	1.048E-01	25	H343	0 0 0 0 0	
6.184E-04	1.244E-01	30	B324	0 0 0 0 0	
6.460E-04	1.300E-01	30	B324	0 0 0 0 0	
1.988E-04	4.000E-02	30	D089	2 2 0 0 0	
6.520E-04	1.312E-01	30	H343	0 0 0 0 0	
1.988E-04	4.000E-02	30	M161	1 0 0 0 1	
7.860E-04	1.582E-01	35	H343	0 0 0 0 0	
8.990E-04	1.809E-01	40	H343	0 0 0 0 0	
1.006E-03	2.024E-01	45	H343	0 0 0 0 0	
1.988E-04	4.000E-02	ns	H042	0 0 0 0 1	
2.783E-04	5.600E-02	ns	M110	0 0 0 0 0	EFG

2776. $C_{12}H_{11}N_3$
C.I. Solvent yellow 1
p-Aminoazobenzene
4-Aminoazobenzene
4-Amino-azobenzol
RN: 60-09-3 **MP** (°C)**:** 125
MW: 197.24 **BP** (°C)**:** >360

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.591E-04	1.300E-01	18	F300	1 0 0 0 1	
1.500E-04	2.959E-02	25	B333	0 0 0 0 0	
2.484E-04	4.900E-02	37	H120	1 1 1 1 1	normal saline
5.510E-04	1.087E-01	60	B198	1 2 1 1 2	
1.041E-03	2.053E-01	71.80	B198	1 2 1 1 2	
1.907E-03	3.761E-01	84.10	B198	1 2 1 1 2	
3.431E-03	6.767E-01	97.40	B198	1 2 1 1 2	

2777. $C_{12}H_{11}N_3$
Diazoaminobenzene
1,3-Diphenyltriazene
Anilinoazobenzene
N-(Phenylazo)aniline
RN: 136-35-6 **MP** (°C)**:** 98.0
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-03	4.998E-01	rt	D021	0 0 1 1 0	

2778. $C_{12}H_{11}N_3O_3$
Orotic acid benzylamide
Orotamide, *N*-benzyl-
RN: 13156-36-0 **MP** (°C)**:** 260–263
MW: 245.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-02	1.128E+01	–4	N018	0 0 0 0 0	
8.700E-02	2.134E+01	16	N018	0 0 0 0 0	
1.180E-01	2.894E+01	25	N018	0 0 0 0 0	

2779. $C_{12}H_{11}O_4P$
Diphenyl phosphate
Phosphoric acid, diphenyl ester
RN: 838-85-7 **MP** (°C)**:** 63
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.08E-03	>2.70E-01	24	H116	2 1 0 0 0	

2780. $C_{12}H_{12}$
1,5-Dimethylnaphthalene
RN: 571-61-9 **MP** (°C)**:** 81
MW: 156.23 **BP** (°C)**:** 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.754E-05	2.740E-03	25	E004	2 1 2 2 2	
2.163E-05	3.380E-03	25	M064	1 1 2 2 2	
2.160E-05	3.375E-03	25	M342	1 0 1 1 2	
2.163E-05	3.380E-03	ns	M344	0 0 0 0 2	

2781. $C_{12}H_{12}$
1-Ethylnaphthalene
RN: 1127-76-0 **MP** (°C)**:** –15
MW: 156.23 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-05	8.124E-03	10	S076	2 2 2 2 1	
5.200E-05	8.124E-03	14	S076	2 2 2 2 1	
6.400E-05	9.999E-03	20	S076	2 2 2 2 1	
6.849E-05	1.070E-02	25	M064	1 1 2 2 2	
6.850E-05	1.070E-02	25	M342	1 0 1 1 2	
6.400E-05	9.999E-03	25	S076	2 2 2 2 1	
6.849E-05	1.070E-02	ns	M344	0 0 0 0 2	

2782. $C_{12}H_{12}$
2,3-Dimethylnaphthalene
RN: 581-40-8 **MP** (°C)**:** 103
MW: 156.23 **BP** (°C)**:** 269

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.274E-05	1.990E-03	25	E004	2 1 2 2 2	
1.920E-05	3.000E-03	25	M064	1 1 2 2 1	
1.920E-05	3.000E-03	25	M342	1 0 1 1 2	
1.920E-05	3.000E-03	ns	M344	0 0 0 0 1	

2783. $C_{12}H_{12}$
1,3-Dimethylnaphthalene
RN: 575-41-7 **MP** (°C)**:** –5
MW: 156.23 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-05	8.000E-03	25	M064	1 1 2 2 1	
5.120E-05	7.999E-03	25	M342	1 0 1 1 2	
5.121E-05	8.000E-03	ns	M344	0 0 0 0 1	

2784. $C_{12}H_{12}$
2,6-Dimethylnaphthalene
RN: 581-42-0 **MP** (°C)**:** 109
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-05	2.000E-03	25	M064	1 1 2 2 1	
1.280E-05	2.000E-03	25	M342	1 0 1 1 2	
1.280E-05	2.000E-03	ns	M344	0 0 0 0 1	

2785. $C_{12}H_{12}$
2-Ethylnaphthalene
RN: 939-27-5 **MP** (°C)**:** –7.4
MW: 156.23 **BP** (°C)**:** 251.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.895E-05	9.210E-03	20	B356	0 0 0 0 0	
5.121E-05	8.000E-03	25	E004	2 1 2 2 2	

2786. $C_{12}H_{12}$
1,4-Dimethylnaphthalene
RN: 571-58-4 **MP** (°C)**:** 7.6
MW: 156.23 **BP** (°C)**:** 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.544E-05	7.100E-03	4	D351	1 2 1 1 2	
4.744E-05	7.412E-03	10	D351	1 2 1 1 2	
6.081E-05	9.500E-03	20	B318	0 0 0 0 0	EFG
6.062E-05	9.470E-03	20	B356	0 0 0 0 0	
6.167E-05	9.634E-03	25	D351	1 2 1 1 2	
7.297E-05	1.140E-02	25	M064	1 1 2 2 2	
7.300E-05	1.140E-02	25	M342	1 0 1 1 1	
7.944E-05	1.241E-02	40	D351	1 2 1 1 2	
7.297E-05	1.140E-02	ns	M344	0 0 0 0 2	

2787. $C_{12}H_{12}ClNO$
2-Chloro-*N*-(1-methyl-2-propynyl)acetanilide
Basamaize
RN: 35846-47-0 **MP** (°C)**:** 40
MW: 221.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	5.000E-01	20	B200	1 0 0 0 0	

2788. $C_{12}H_{12}N_2$
Benzidine
Benzidin
p-Diaminobiphenyl
RN: 92-87-5 **MP** (°C)**:** 117
MW: 184.24 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E-03	3.599E-01	24	H106	1 0 2 2 2	
1.954E-03	3.600E-01	24	M303	1 0 1 1 2	pH 5.9
2.712E-03	4.998E-01	25	B019	1 0 1 2 0	
2.822E-03	5.200E-01	25	B068	2 0 1 1 1	
2.700E-04	4.975E-02	25	H091	1 2 2 2 1	*sic*
1.465E-03	2.699E-01	rt	N015	0 0 2 2 2	

2789. $C_{12}H_{12}N_2$
m-Benzidine
3-Benzidine
RN: 2050-89-7 **MP** (°C)**:** 117
MW: 184.24 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.970E-02	1.100E+01	100	F300	1 0 0 0 1	

2790. $C_{12}H_{12}N_2OS$
2,4-Dimethyl-5-carboxanilidothiazole
G-696
RN: 21452-18-6 **MP** (°C)**:** 141
MW: 232.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-02	2.454E+00	25	M061	1 0 0 0 2	

2791. $C_{12}H_{12}N_2O_2S$
Dapsone
4,4′-Diaminodiphenyl sulphone
RN: 80-08-0 **MP** (°C)**:** 175
MW: 248.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.638E-04	1.400E-01	25	P351	0 0 0 0 0	pH 7.4
6.444E-04	1.600E-01	25	P351	0 0 0 0 0	
1.530E-03	3.800E-01	37	L037	1 2 2 1 1	
4.027E-04	1.000E-01	ns	K444	0 0 0 0 0	

2792. $C_{12}H_{12}N_2O_2S$
Sulfabenz
Sulfanilid
RN: 127-77-5 **MP** (°C)**:**
MW: 248.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.819E-02	7.000E+00	100	F300	1 0 0 0 0	

2793. $C_{12}H_{12}N_2O_3$
Nalidixic acid
NegGRAM
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid
Nalidic acid
RN: 389-08-2 **MP** (°C)**:** 228
MW: 232.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.306E-04	1.000E-01	23	G098	1 0 0 0 0	
7.079E-01	1.644E+02	37	O307	1 0 1 2 1	pH 2, EFG
4.306E-04	1.000E-01	ns	K444	0 0 0 0 0	

2794. $C_{12}H_{12}N_2O_3$
Phenobarbital
5-Ethyl-5-phenylbarbituric acid
Phenylethylmalonylurea
RN: 50-06-6 **MP** (°C)**:** 176
MW: 232.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-03	9.243E-01	15	H018	0 0 0 0 0	
3.680E-03	8.546E-01	15	S149	1 2 2 1 2	anhydrate

(*continued*)

2794. $C_{12}H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-03	7.385E-01	15	S149	1 2 2 1 2	hydrate
4.736E-03	1.100E+00	20	I009	1 2 2 1 1	EFG, 0.005M HCl
3.789E-03	8.800E-01	20	J030	1 2 2 2 1	
4.521E-03	1.050E+00	20	K143	1 2 2 2 2	form II
5.081E-03	1.180E+00	20	K143	1 2 2 2 2	form III
3.143E-03	7.300E-01	20	N023	1 2 2 1 1	hydrate
4.866E-03	1.130E+00	20	N023	1 2 2 1 2	anhydrate
3.920E-03	9.104E-01	20	S149	1 2 2 1 2	hydrate
4.510E-03	1.047E+00	20	S149	1 2 2 1 2	anhydrate
4.731E-03	1.099E+00	25	A023	1 0 0 1 1	
5.167E-03	1.200E+00	25	B011	2 0 0 1 0	
4.994E-03	1.160E+00	25	B065	1 1 1 1 0	
5.590E-03	1.298E+00	25	E011	2 1 1 2 1	
7.737E-03	1.797E+00	25	E011	2 1 1 2 1	pH 7.0
3.078E-02	7.149E+00	25	E011	2 1 1 2 1	pH 8.0
4.731E-03	1.099E+00	25	F009	2 2 2 2 0	EFG
4.600E-03	1.068E+00	25	G003	1 1 1 1 1	pH 4.7
2.734E-03	6.350E-01	25	H005	1 0 1 2 2	
5.161E-03	1.199E+00	25	K010	2 0 0 1 1	
6.114E-03	1.420E+00	25	K143	1 2 2 2 2	form III
5.512E-03	1.280E+00	25	K143	1 2 2 2 2	form II
4.650E-03	1.080E+00	25	L032	2 1 2 0 2	
4.790E-03	1.112E+00	25	M056	2 2 2 2 2	
5.684E-03	1.320E+00	25	N023	1 2 2 1 2	anhydrate
4.995E-03	1.160E+00	25	N023	1 2 2 1 2	hydrate
6.020E-03	1.398E+00	25	P006	2 0 2 2 1	
4.306E-03	1.000E+00	25	P015	0 0 0 0 0	
4.761E-03	1.106E+00	25	P350	0 0 0 0 0	intrinsic
4.830E-03	1.122E+00	25	S149	1 2 2 1 2	hydrate
5.320E-03	1.236E+00	25	S149	1 2 2 1 2	anhydrate
5.170E-03	1.201E+00	25	V033	2 0 1 1 2	
5.200E-03	1.208E+00	25.00	T303	1 0 0 0 1	
6.700E-03	1.556E+00	30	A065	2 0 2 2 1	
6.310E-03	1.465E+00	30	H018	0 0 0 0 0	
6.000E-03	1.393E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
6.100E-03	1.417E+00	30	K108	1 2 2 0 1	
6.502E-03	1.510E+00	30	K143	1 2 2 2 2	form II
7.148E-03	1.660E+00	30	K143	1 2 2 2 2	form III
6.071E-03	1.410E+00	30	N023	1 2 2 1 2	hydrate
6.502E-03	1.510E+00	30	N023	1 2 2 1 2	anhydrate
6.020E-03	1.398E+00	30	O321	0 0 0 0 0	
6.000E-03	1.393E+00	30	O321	0 0 0 0 0	
8.612E-03	2.000E+00	32	M157	2 0 1 1 0	EFG
7.737E-03	1.797E+00	35	A023	1 0 0 1 2	
7.700E-03	1.788E+00	35	S149	1 2 2 1 2	hydrate
7.750E-03	1.800E+00	35	S149	1 2 2 1 2	anhydrate
8.500E-03	1.974E+00	35.00	T303	1 0 0 0 1	

(*continued*)

2794. $C_{12}H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.923E-03	1.840E+00	37	J030	1 2 2 2 2	
8.000E-03	1.858E+00	37	K121	1 2 1 2 0	0.1N HCl
9.023E-03	2.096E+00	40	A023	1 0 0 1 2	
9.000E-02	2.090E+01	40	N008	1 0 1 1 2	*sic*
1.055E-02	2.450E+00	45	S149	1 2 2 1 2	anhydrate
1.108E-02	2.573E+00	45	S149	1 2 2 1 2	hydrate
1.130E-02	2.624E+00	45.00	T303	1 0 0 0 2	
1.266E-02	2.940E+00	50	S149	1 2 2 1 2	anhydrate
1.506E-02	3.498E+00	50	S149	1 2 2 1 2	hydrate
1.698E-02	3.943E+00	55	S149	1 2 2 1 2	hydrate
1.499E-02	3.481E+00	55	S149	1 2 2 1 2	anhydrate
1.033E-02	2.400E+00	60	I009	1 2 2 1 1	EFG, 0.005M HCl
4.306E-03	1.000E+00	ns	K444	0 0 0 0 0	
4.177E-03	9.700E-01	ns	T003	0 0 0 0 2	

2795. $C_{12}H_{12}N_2O_6S_2$
Benzidine-2,2′-disulfonic acid
Benzidin-disulfosaeure-(2,2′)
RN: 117-61-3 **MP** (°C)**:**
MW: 344.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-03	8.000E-01	25	F300	1 0 0 0 0	

2796. $C_{12}H_{12}N_2S$
Thiopyrine
1-Phenyl-2,3-dimethyl-3-pyrazoline-5-thione
RN: 5702-69-2 **MP** (°C)**:** 166
MW: 216.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-02	1.428E+01	ns	D087	0 2 0 0 2	

2797. $C_{12}H_{12}N_4O_3$
Benznidazole
2-Nitro-*N*-(phenylmethyl)-imidazole-1-acetamide
RN: 22994-85-0 **MP** (°C)**:**
MW: 260.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	ns	K444	0 0 0 0 0	

2798. $C_{12}H_{12}N_4O_3S$
*N*4-Acetylsulfapyrazine
*N*4-Acetylsulphapyrazine
RN: 5433-91-0 **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2799. $C_{12}H_{12}N_4O_3S$
*N*4-Acetyl sulfadiazine
*N*4-Acetylsulfadiazine
Acetyl sulfadiazine
2-*N*4-Acetylsulfanilamidopyrimidine
RN: 127-74-2 **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
	1.500E-01	37	F075	1 0 2 2 2	
7.200E-04	2.105E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
6.842E-04	2.000E-01	37	L091	1 0 0 0 1	pH 5.5
8.723E-04	2.550E-01	37	M057	1 0 0 0 2	pH 5.5
5.131E-04	1.500E-01	37	R045	1 2 1 1 1	

2800. $C_{12}H_{12}N_6O_6$
TMPPT
1,3,7,9-Tetramethylpyrimido(5,4-γ) pteridine-2,4,6,8(1H,3H,7H,9H)-tetrone
RN: **MP** (°C)**:**
MW: 336.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-04	1.298E-01	25	K008	1 1 0 1 0	EFG
3.900E-04	1.311E-01	25	K009	1 2 1 1 0	EFG

2801. $C_{12}H_{12}O_6$
Benzoic acid, 2-(acetyloxy)-, (acetyloxy)methyl ester
Salicylic acid acetate, hydroxymethyl ester acetate
RN: 32620-68-1 **MP** (°C)**:** oil
MW: 252.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.634E-03	2.430E+00	21	N335	0 0 0 0 0	

2802. $C_{12}H_{13}ClN_2O$
Buturon
3-(*para*-Chlorophenyl)-1-methyl-1-(1-methyl-2-propynyl) urea
Urea, *N′*-(4-chlorophenyl)-*N*-methyl-*N*-(1-methyl-2-propynyl)
Eptapur
RN: 3766-60-7 **MP** (°C)**:** 145.5
MW: 236.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.267E-04	3.000E-02	20	G036	1 0 0 0 1	
1.267E-04	3.000E-02	20	M161	1 0 0 0 1	

2803. $C_{12}H_{13}ClN_4$
Pyrimethamine
RN: 58-14-0 **MP** (°C)**:** 238
MW: 248.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E-05	1.000E-02	ns	K444	0 0 0 0 0	

2804. $C_{12}H_{13}I_3N_2O_2$
Iopodic acid
Ipodic acid
RN: 5587-89-3 **MP** (°C)**:**
MW: 597.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.027E-03	1.810E+00	ns	H055	0 0 0 0 0	

2805. $C_{12}H_{13}I_3N_2O_3$
Iocetamic acid
N-(3-Amino-2,4,6-triiodophenyl)-3-acetamido-2-methylpropionic acid
Cholebrine
MP 620
DRC 1201
RN: 16034-77-8 **MP** (°C)**:** 224
MW: 613.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.610E-03	5.286E+00	37	J016	1 0 0 0 2	pH 7.4

2806. $C_{12}H_{13}NO_2$
Methsuximide
Celontin
N-Methyl-α-methyl-α-phenylsuccinimide
RN: 77-41-8 **MP** (°C)**:** 52–53
MW: 203.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.378E-02	2.800E+00	25	P061	0 0 0 0 0	

2807. $C_{12}H_{13}NO_2S$
Carboxin
2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin
Vitavax
RN: 5234-68-4 **MP** (°C)**:** 94
MW: 235.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.225E-04	1.700E-01	25	M061	1 0 0 0 2	
7.225E-04	1.700E-01	25	M161	1 0 0 0 2	

2808. $C_{12}H_{13}NO_2S$
4-Thiazolidinecarboxylic acid, 2-(4-ethenylphenyl)-
RN: 256235-52-6 **MP** (°C)**:**
MW: 235.31 **BP** (°C)**:** 464.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	8.706E-01	21	B414	1 0 0 1 1	partial decomposition

2809. $C_{12}H_{13}NO_3$
Azetidine, 1-[(benzoyloxy)acetyl]-
RN: 115178-66-0 **MP** (°C)**:** 74.5
MW: 219.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-02	5.400E+00	22	N317	1 1 2 1 2	

2810. $C_{12}H_{13}NO_3$
Crotonyl acetaminophen
Crotonic acid, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, crotonate (ester)
RN: 20675-24-5 **MP** (°C)**:** 146-147
MW: 219.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.961E-03	4.300E-01	37	D029	0 0 0 0 0	

2811. $C_{12}H_{13}NO_4$
Acetamide, *N*-acetyl-2-(benzoyloxy)-*N*-methyl-
RN: 115178-80-8 **MP** (°C)**:**
MW: 235.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	N317	1 1 2 1 2	

2812. $C_{12}H_{13}NO_4S$
Plantvax
2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin-4,4-dioxide
Oxycarboxin
RN: 5259-88-1 **MP** (°C)**:** 128.7
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.741E-03	1.000E+00	25	M161	1 0 0 0 0	
3.741E-03	1.000E+00	ns	M061	0 0 0 0 2	

2813. $C_{12}H_{13}NO_4S_2$
4-Ethylsulfonylnaphthalene-1-sulfonamide
ENS
4-ENS
RN: 842-00-2 **MP** (°C)**:**
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.775E-04	1.130E-01	c	K042	2 2 2 2 2	

2814. $C_{12}H_{13}NO_5$
Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-
RN: 106231-64-5 **MP** (°C)**:** 160.5
MW: 251.24 **BP** (°C)**:** 475.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.572E-03	1.400E+00	22	B427	1 0 0 1 1	in 0.01M HCl
5.572E-03	1.400E+00	22	N317	1 1 2 1 2	

2815. $C_{12}H_{13}NO_5$
Succinyl acetaminophen
Butanedioic acid, mono[4-(acetylamino)phenyl] ester
Acetanilide, 4′-hydroxy-, hydrogen succinate ester
RN: 20675-25-6 **MP** (°C)**:** 145.5-146.5
MW: 251.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-02	6.500E+00	37	D029	0 0 0 0 0	

2816. $C_{12}H_{13}NO_6$
Carbobenzoxydiglycine
RN: **MP** (°C)**:**
MW: 267.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-03	6.500E-01	25.1	N026	0 0 0 0 0	
2.804E-03	7.494E-01	25.1	N027	1 1 2 2 2	

2817. $C_{12}H_{13}N_3O_2$
Isocarboxazid
Marplan
RN: 59-63-2 **MP** (°C)**:**
MW: 231.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-03	8.000E-01	25	R024	0 0 0 0 0	

2818. $C_{12}H_{13}N_3O_2S$
*N*1-Methyl-*N*1-2-pyridyl-sulfanilamide
*N*1-Methyl-*N*1-(2-pyridyl)sulfanilamide
RN: 51543-29-4 **MP** (°C)**:**
MW: 263.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.740E-03	1.248E+00	37	K095	2 0 0 0 2	intrinsic

2819. $C_{12}H_{13}N_3O_3S_2$
Methyl acetyl sulfathiazole
Sulfathiazol methyle acetyle
RN: **MP** (°C)**:**
MW: 311.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.248E-04	7.000E-02	37	D084	1 0 1 0 0	

2820. $C_{12}H_{13}N_3O_4S$
Acetylsulfamethoxazole
Acetanilide, 4′-[(5-methyl-3-isoxazolyl)sulfamoyl]-
4′-Acetyl-3-sulfa-5-methylisoxazole
RN: 21312-10-7 **MP** (°C)**:**
MW: 295.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.573E-04	7.600E-02	37	H120	1 1 1 1 1	normal saline

2821. $C_{12}H_{14}ClNO_2$
Clomazone
Command
Dimethazone
Fenoxan
FMC 57020
Gamit
RN: 81777-89-1 **MP** (°C)**:** 25
MW: 239.70 **BP** (°C)**:** 275.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.101E+00	ns	S460	0 0 0 0 0	

2822. $C_{12}H_{14}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-butyl ester
2,4-Dichlorophenoxyacetic acid butyl ester
RN: 94-80-4 **MP** (°C)**:**
MW: 277.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.495E-05	1.523E-02	ns	M120	0 0 1 1 2	

2823. $C_{12}H_{14}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *sec*-butyl ester

RN: 94-79-1 **MP** (°C)**:**
MW: 277.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.252E-05	1.733E-02	ns	M120	0 0 1 1 2	

2824. $C_{12}H_{14}Cl_3O_4P$

Chlorfenvinphos
2-Chloro-1-(2,4-dichlorophenyl)ethenyl phosphoric acid, diethyl ester
Dermaton
Birlanex
Birlane
Steladone

RN: 470-90-6 **MP** (°C)**:**
MW: 359.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
4.074E-04	1.465E-01	20	B179	0 0 0 0 0	
3.449E-04	1.240E-01	20	B300	2 1 1 1 2	
3.449E-04	1.240E-01	20	B324	0 0 0 0 0	
3.448E-04	1.240E-01	20	B324	0 0 0 0 0	
3.893E-04	1.400E-01	20	F311	1 2 2 2 1	
4.033E-04	1.450E-01	20	M061	1 0 0 0 2	
4.033E-04	1.450E-01	23	M161	1 0 0 0 2	
2.976E-04	1.070E-01	30	B324	0 0 0 0 0	
2.975E-04	1.070E-01	30	B324	0 0 0 0 0	

2825. $C_{12}H_{14}NO_4PS$

Ditalimfos
O,*O*-Diethyl (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl) phosphonothioate
Laptran
Plondrel

RN: 5131-24-8 **MP** (°C)**:** 83.5
MW: 299.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.444E-04	1.330E-01	rt	M161	0 0 0 0 2	

2826. $C_{12}H_{14}N_2O_2$
Primidone
5-Ethyldihydro-5-phenyl-4,6(1H,5H)-pyrimidinedione
Desoxyphenobarbitone
2-Deoxyphenobarbital
RN: 125-33-7 **MP** (°C)**:** 281.5
MW: 218.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-03	4.700E-01	25	C437	0 0 0 0 0	Average
2.200E-03	4.802E-01	30	K108	1 2 2 0 1	
2.747E-03	5.996E-01	37	P061	0 0 0 0 0	
2.291E-03	5.000E-01	rt	D025	0 0 0 0 0	

2827. $C_{12}H_{14}N_2O_4$
Acetamide, *N*-(2-amino-2-oxoethyl)-2-(benzoyloxy)-*N*-methyl-
RN: 106231-62-3 **MP** (°C)**:** 101.5
MW: 250.26 **BP** (°C)**:** 496.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-01	3.020E+01	22	B427	1 0 0 1 1	in 0.01M HCl
1.207E-01	3.020E+01	22	N317	1 1 2 1 2	

2828. $C_{12}H_{14}N_2O_4$
Propanamide, 2-[[(benzoyloxy)acetyl]amino]-
RN: 115193-30-1 **MP** (°C)**:** 201.5
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	4.800E-01	22	N317	1 1 2 1 2	

2829. $C_{12}H_{14}N_2O_5$
2-Cyclohexyl-4,6-dinitrophenol
Dinex
4,6-Dinitro-2-cyclohexylphenol
2,4-Dinitro-6-cyclohexylphenol
RN: 131-89-5 **MP** (°C)**:** 106
MW: 266.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.634E-05	1.500E-02	25	M061	1 0 0 0 1	pH 6.5
6.760E-06	1.800E-03	25	M061	1 0 0 0 1	pH 1

2830. $C_{12}H_{14}N_2O_6$
Dinoseb acetate
Aretit
RN: 2813-95-8 **MP** (°C)**:** 26.5
MW: 282.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.794E-03	2.200E+00	rt	M161	0 0 0 0 1	

2831. $C_{12}H_{14}N_4O_2S$
6-Sulfanilamido-2,4-dimethylpyrimidine
6-Sulfanilamido-2,4-dimethylpyrimidin
Sulfisomidine
Sulphasomidine
RN: 515-64-0 **MP** (°C)**:** 243.0
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.965E-03	1.382E+00	25	M319	2 1 1 1 2	
6.862E-03	1.910E+00	37	K086	1 0 0 0 2	
5.802E-03	1.615E+00	ns	B133	0 2 0 1 2	pH 7.4
1.075E-02	2.991E+00	ns	M141	0 0 0 0 0	

2832. $C_{12}H_{14}N_4O_2S$
Sulfamethazine
Sulfadimezine
2-Sulfanilamido-4,6,-dimethylpyrimidine
RN: 57-68-1 **MP** (°C)**:** 176
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.317E-03	1.480E+00	20	F073	1 2 2 2 2	
1.544E-03	4.298E-01	20	L058	1 0 1 1 2	
1.893E-03	5.269E-01	20	O032	1 0 0 0 2	
1.424E-03	3.963E-01	24	N021	2 0 1 2 2	pH 5.6
1.600E-03	4.453E-01	25	M440	0 0 0 0 0	
5.389E-03	1.500E+00	29	C049	0 0 0 0 0	
2.695E-03	7.500E-01	37	L091	1 0 0 0 1	pH 5.5
6.862E-03	1.910E+00	37	M057	1 0 0 0 2	pH 5.5
2.414E-03	6.720E-01	37	S192	1 0 1 1 2	pH 6.0
2.299E-03	6.400E-01	38	K006	1 0 0 0 1	
1.185E-03	3.299E-01	ns	L044	0 0 0 0 2	

2833. $C_{12}H_{14}N_4O_2S.0.5H_2O$
Sulphamethazine (hemihydrate)
Sulfamethazine hemihydrate
RN: 57-68-1 **MP** (°C)**:**
MW: 287.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.786E-03	1.950E+00	37	R044	0 0 0 0 0	

2834. $C_{12}H_{14}N_4O_2S$
2-Sulfanilamido-4,5-dimethylpyrimidine
RN: 4462-43-5 **MP** (°C)**:** 225.7
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.186E-04	2.000E-01	29	C049	0 0 0 0 0	

2835. $C_{12}H_{14}N_4O_2S$
2-Sulfanilylamino-4-ethylpyrimidine
RN: 2276-96-2 **MP** (°C)**:**
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.180E-04	1.720E-01	37	R076	1 2 0 0 2	

2836. $C_{12}H_{14}N_4O_3S_2$
Acetyl sulfaethylthiadiazole
Acetamide, *N*-[4-[[(5-ethyl-1,3,4-thiadiazol-2-yl)amino]sulfonyl]phenyl]-
RN: 1037-51-0 **MP** (°C)**:**
MW: 326.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E-03	1.620E+00	37	B046	1 0 2 2 2	pH 4.6

2837. $C_{12}H_{14}N_4O_3S$
Sulfamethomidine
Sulphamethomidine
RN: 3772-76-7 **MP** (°C)**:** 146.0
MW: 294.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.864E-03	8.430E-01	ns	B133	0 2 0 1 2	pH 7.4
2.884E-03	8.489E-01	ns	R427	0 0 0 0 0	

2838. $C_{12}H_{14}N_4O_3S$
2-Sulfanilamido-4-ethoxypyrimidine
RN: 71138-72-2 **MP** (°C)**:**
MW: 294.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-04	5.300E-02	37	R046	1 2 1 1 2	

2839. $C_{12}H_{14}N_4O_4S$
Sulfadimethoxine
Sulphadimethoxine
RN: 122-11-2 **MP** (°C)**:** 202.0
MW: 310.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.492E-04	4.630E-02	37	W055	1 2 0 1 2	
1.105E-03	3.430E-01	ns	B133	0 2 0 1 2	pH 7.4

2840. $C_{12}H_{14}N_4O_4S$
Sulfadoxine
Sulformethoxine
Sulforthomidine
4-Amino-*N*-(5,6-dimethoxy-4-pyrimidinyl)benzenesulfonamide
Fanzil
Fanasil
RN: 2447-57-6 **MP** (°C)**:** 190–194
MW: 310.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.761E-04	2.098E-01	ns	R427	0 0 0 0 0	

2841. $C_{12}H_{14}O_4$
Diethyl phthalate
Ethyl phthalate
Di-ethyl phthalate
Phthalic acid ethyl ester
Phthalsaeure-diaethyl ester
RN: 84-66-2 **MP** (°C)**:** –40.5
MW: 222.24 **BP** (°C)**:** 296.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.495E-03	9.990E-01	20	F070	1 0 0 0 0	
4.180E-03	9.290E-01	20	L300	2 1 0 2 2	
1.793E-02	3.984E+00	20.00	D343	0 0 0 0 0	
5.399E-03	1.200E+00	25	F067	1 0 2 2 2	
4.500E-03	1.000E+00	25	F300	1 0 0 0 0	

2842. $C_{12}H_{14}O_4$
Trimethylacetyl salicylate
Salicylic acid, pivalate
2-Carboxyphenyl pivalate
RN: 2704-58-7 **MP** (°C)**:**
MW: 222.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.730E-04	2.162E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.74, intrinsic

2843. $C_{12}H_{14}O_4$
Diethyl *o*-phthalate
RN: **MP** (°C)**:** –40 C
MW: 222.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-03	8.040E-01	25	S417	0 0 0 0 0	

2844. $C_{12}H_{15}ClNO_4PS_2$
Phosalone
Diethyl *S*-((6-chloro-2-oxobenzoxazolin-3-yl)methyl) phosphorodithioate
Rubitox
Benzophosphate
RN: 2310-17-0 **MP** (°C)**:**
MW: 367.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B300	2 2 1 1 2	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
5.845E-06	2.150E-03	20	C053	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
5.845E-06	2.150E-03	ns	F071	0 1 2 1 2	
2.719E-05	1.000E-02	rt	M161	0 0 0 0 1	

2845. $C_{12}H_{15}ClO_3$
Clofibrate
2-(*p*-Chlorophenoxy)-2-methylpropionic acid ethyl ester
Abitrate
Atromid S
RN: 637-07-0 **MP** (°C)**:**
MW: 242.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.708E-02	rt	G093	0 1 1 1 2	

2846. $C_{12}H_{15}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-propanoate
5′-Propionyl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-propionate
RN: 84043-25-4 **MP** (°C)**:** 167.5
MW: 410.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E+03	1.427E+06	25	N332	0 0 0 0 0	pH 7.4

2847. $C_{12}H_{15}NO$
n-Propylcinnamamide
Cinnamamide, *N*-propyl-
2-Propenamide, 3-phenyl-*N*-propyl-
RN: 6329-15-3 **MP** (°C)**:**
MW: 189.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.353E-01	ns	H350	0 0 0 0 0	

2848. $C_{12}H_{15}NO_3$
Acetamide, *N*-[2-(benzoyloxy)ethyl]-*N*-methyl-
RN: 57440-16-1 **MP** (°C)**:**
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	3.130E+01	22	N317	1 1 2 1 2	

2849. $C_{12}H_{15}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-propyl-
RN: 106231-51-0 **MP** (°C)**:** 89.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.893E-03	6.400E-01	22	B427	1 0 0 1 1	in 0.01M HCl
2.893E-03	6.400E-01	22	N317	1 1 2 1 2	

2850. $C_{12}H_{15}NO_3$
Propanamide, 3-(benzoyloxy)-*N*,*N*-dimethyl-
RN: 115178-77-3 **MP** (°C)**:**
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.955E-02	1.760E+01	22	N317	1 1 2 1 2	

2851. $C_{12}H_{15}NO_3$
Carbofuran
2,3-Dihydro-2,2-dimethyl-7-benzofuranol methylcarbamate
Crisfuran
Furadanx
Curaterr
RN: 1563-66-2 **MP** (°C)**:** 152
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-03	2.909E-01	10	B324	0 0 0 0 0	
1.315E-03	2.910E-01	10	B324	0 0 0 0 0	
1.446E-03	3.199E-01	19	B169	2 1 1 1 1	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
3.164E-03	7.000E-01	25	M161	1 0 0 0 2	
1.695E-03	3.750E-01	30	B324	0 0 0 0 0	
1.694E-03	3.749E-01	30	B324	0 0 0 0 0	
1.446E-03	3.200E-01	ns	V414	0 0 0 0 0	

2852. $C_{12}H_{15}NO_3$
Acetaminophen butyrate
Butyryl acetaminophen
Butanoic acid, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, butyrate
RN: 14771-98-3 **MP** (°C)**:** 140
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	3.300E-01	25	B010	1 1 1 1 0	
2.441E-03	5.400E-01	37	D029	0 0 0 0 0	

2853. $C_{12}H_{15}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-(1-methylethyl)-
RN: 115193-27-6 **MP** (°C)**:** 129.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-03	4.100E-01	22	N317	1 1 2 1 2	

2854. $C_{12}H_{15}NO_4$
Isopropyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl 1-methylethyl ester
Acetanilide, 4′-hydroxy-, isopropyl carbonate
RN: 17239-27-9 **MP** (°C)**:** 131.5–132
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.636E-03	1.100E+00	37	D029	0 0 0 0 0	

2855. $C_{12}H_{15}NO_4$
Acetamide, 2-(benzoyloxy)-*N*-(2-hydroxyethyl)-*N*-methyl-
RN: 106231-59-8 **MP** (°C)**:** 79
MW: 237.26 **BP** (°C)**:** 428.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.135E-02	1.930E+01	22	B427	1 0 0 1 1	in 0.01M HCl
8.135E-02	1.930E+01	22	N317	1 1 2 1 2	

2856. $C_{12}H_{15}NO_4$
O-(Butyryloxymethyl) salicylamide
O-Butyryloxymethyl salicylamide
Butanoic acid, [2-(aminocarbonyl)phenoxy]methyl ester
RN: 103951-39-9 **MP** (°C)**:** 57
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	2.500E+00	23	B328	1 2 2 1 1	pH 4.0
1.054E-02	2.500E+00	23	B328	0 0 0 0 0	

2857. $C_{12}H_{15}NO_5$
Benzoic acid, 2-hydroxy-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl ester
N-Methyl-*N*-carbamoylmethyl glycolamide salicylate
RN: 114665-09-7 **MP** (°C)**:** 92.5
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.300E+00	21	B331	1 2 2 1 0	pH 7.4
2.488E-02	6.300E+00	21	B331	0 0 0 0 0	

2858. $C_{12}H_{15}NO_6$
Ethonyphenyl tartramic acid
RN: **MP** (°C)**:** 201
MW: 269.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.989E+00	14	C069	1 2 0 1 2	

2859. $C_{12}H_{15}N_2O_3PS$
Phoxim
4-Ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile 4-sulfide
Baythion
Sebacil
Volation
RN: 14816-18-3 **MP** (°C)**:**
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-05	3.300E-03	10	B324	0 0 0 0 0	
1.106E-05	3.299E-03	10	B324	0 0 0 0 0	
1.374E-05	4.099E-03	20	B300	2 1 1 1 2	
1.374E-05	4.099E-03	20	B324	0 0 0 0 0	
1.374E-05	4.100E-03	20	B324	0 0 0 0 0	

(*continued*)

2859. $C_{12}H_{15}N_2O_3PS$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-05	7.000E-03	20	M161	1 0 0 0 0	
1.643E-05	4.901E-03	30	B324	0 0 0 0 0	
1.643E-05	4.900E-03	30	B324	0 0 0 0 0	
1.374E-05	4.099E-03	ns	S460	0 0 0 0 0	

2860. $C_{12}H_{15}N_2O_3PS$

Quinalphos
Diethyl *O*-(2-quinoxalyl) phosphorothioate
Diethquinalphion
Bayrusil
Ekalux

RN: 13593-03-8 **MP** (°C)**:** 33.5
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.375E-05	2.200E-02	24	M161	1 0 0 0 1	

2861. $C_{12}H_{15}N_3O_2S$

1-Methyl-2-sulfanilamide-1,2-dihydropyridine
Benzenesulfonamide, 4-amino-*N*-(1,2-dihydro-1-methyl-2-pyridinyl)-

RN: 51543-30-7 **MP** (°C)**:**
MW: 265.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-03	9.791E-01	37	K095	2 0 0 0 2	intrinsic

2862. $C_{12}H_{15}N_3O_2S$

Albendazole
Bilutac
Eskazole
Proftril
Valbazan
Zentel

RN: 54965-21-8 **MP** (°C)**:**
MW: 265.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-06	7.500E-04	209	D426	0 0 0 0 0	
3.769E-05	1.000E-02	ns	K444	0 0 0 0 0	

2863. $C_{12}H_{15}N_3O_3$
Triallyl cyanurate
Cyanursaeure-triallylaether
RN: 101-37-1 **MP** (°C)**:** 26–28
MW: 249.27 **BP** (°C)**:** 119–120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.407E-02	6.000E+00	20	F300	1 0 0 0 0	

2864. $C_{12}H_{15}N_3O_3S$
Albendazole sulphoxide
Ricobendazole
Albendazole oxide
Methoxy-*N*-[5-(propylsulfinyl)benzimidazol-2-yl]carboxamide
Albendazole oxide [BAN:INN]
Carbamic acid
RN: 54029-12-8 **MP** (°C)**:**
MW: 281.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.204E-04	6.200E-02	25	W416	0 0 0 0 0	
1.094E-03	3.079E-01	94.1	D426	0 0 0 0 0	

2865. $C_{12}H_{15}N_3O_6$
1,3,5-Triglycidyl-*S*-triazinetrione
α-TGT
RN: 2451-62-9 **MP** (°C)**:**
MW: 297.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.373E-02	1.300E+01	0	A088	0 0 1 1 1	

2866. $C_{12}H_{15}N_5O_5$
9-[5′-(*O*-Acetyl)-β-D-arabinofuranosyl]adenine ester
Vidarabine 5′-acetate
RN: 65926-28-5 **MP** (°C)**:** 198.0
MW: 309.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.134E-02	6.600E+00	ns	B134	0 1 1 1 1	

2867. $C_{12}H_{15}N_5O_5$
Pivaloyl salicylate
9-(2-*O*-Acetyl-β-D-arabinofuranosyl)adenine
RN: 87970-03-4 **MP** (°C)**:** 195
MW: 309.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-01	9.360E+01	37	B306	1 2 0 1 2	pH 7.3

2868. $C_{12}H_{15}O_3P$
Diallyl phenyl phosphonate
Phosphonic acid, phenyl-, di-2-propenyl ester
RN: 2948-89-2 **MP** (°C)**:**
MW: 238.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-03	3.000E-01	25	B070	1 2 0 1 0	

2869. $C_{12}H_{16}ClNOS$
Orbencarb
Lanray
S-((2-Chlorophenyl)methyl) diethylcarbamothioate
RN: 34622-58-7 **MP** (°C)**:**
MW: 257.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-05	2.400E-02	ns	S460	0 0 0 0 0	

2870. $C_{12}H_{16}ClNOS$
Thiobencarb
S-4-Chlorobenzyl diethylthiocarbamate
Diethylcarbamothioic acid *S*-[(4-chlorophenyl)methyl] ester
4-Chlorobenzyl *N*,*N*-diethylthiocarbamate
RN: 28249-77-6 **MP** (°C)**:**
MW: 257.78 **BP** (°C)**:** 127.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-04	3.000E-02	22	K137	1 1 2 1 0	
1.164E-04	3.001E-02	ns	S460	0 0 0 0 0	

2871. $C_{12}H_{16}Cl_2N_2O$
Neburon
1-Butyl-3-(3,4-dichlorophenyl)-1-methylurea
RN: 555-37-3 **MP** (°C)**:** 101.5
MW: 275.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.744E-05	4.800E-03	20	F311	1 2 2 2 1	
1.744E-05	4.800E-03	24	B185	0 0 0 0 0	
1.744E-05	4.800E-03	24	G036	1 0 0 0 1	
1.744E-05	4.800E-03	24	M061	1 0 0 0 1	
1.744E-05	4.800E-03	24	M161	1 0 0 0 1	
1.744E-05	4.800E-03	25	A039	1 1 0 0 1	
1.744E-05	4.800E-03	25	G099	1 0 0 1 0	
1.744E-05	4.800E-03	ns	K007	0 0 0 0 1	

2872. $C_{12}H_{16}N_2$
Etryptamine
α-Ethyltryptamine
RN: 2235-90-7 **MP** (°C)**:** 97
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.709E-03	5.100E-01	rt	M011	0 0 2 1 1	intrinsic

2873. $C_{12}H_{16}N_2O$
N-(Piperidinomethyl)benzamide
Benzamide, *N*-(1-pyrrolidinylmethyl)-
RN: 92788-60-8 **MP** (°C)**:**
MW: 204.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-03	1.450E+00	22	J037	0 0 0 0 0	

2874. $C_{12}H_{16}N_2O_2$
N,*N*,*N*′,*N*′-Tetramethylterephthalamide
1,4-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 13158-31-1 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.843E+00	4.060E+02	30	K004	1 0 0 0 2	
1.840E+00	4.053E+02	30	K019	1 0 0 0 2	

2875. $C_{12}H_{16}N_2O_2$

N,*N*,*N*′,*N*′-Tetramethylphthalamide
1,2-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 6329-16-4 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.223E+00	7.100E+02	30	K004	1 0 0 0 2	

2876. $C_{12}H_{16}N_2O_2$

N,*N*,*N*′,*N*′-Tetramethylisophthalamide
1,3-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 14334-36-2 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E+00	6.760E+02	30	K004	1 0 0 0 2	
3.070E+00	6.762E+02	30	K019	1 0 0 0 2	

2877. $C_{12}H_{16}N_2O_2S$

4-Thiazolidinecarboxylic acid, 2-[4-(dimethylamino)phenyl]-
4-Thiazolidinecarboxylic acid, 2-(*p*-dimethylaminophenyl)-
RN: 72678-86-5 **MP** (°C)**:**
MW: 252.34 **BP** (°C)**:** 481.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.813E-01	21	B414	1 0 0 1 1	fast decomposition

2878. $C_{12}H_{16}N_2O_3$

Hexobarbital
5-(1-Cyclohexen-1-yl)-1,5-dimethylbarbituric acid
5-(1-Cyclohexenyl)-1,5-dimethylbarbituric acid
Hexabarital
RN: 56-29-1 **MP** (°C)**:** 146
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-03	2.900E-01	20	J030	1 2 2 2 1	
1.840E-03	4.347E-01	25	M056	2 2 2 2 2	
2.000E-03	4.725E-01	30	K108	1 2 2 0 1	
2.709E-03	6.400E-01	37	J030	1 2 2 2 1	

2879. $C_{12}H_{16}N_2O_3$
Carbetamide
N-Ethyl-2-(((phenylamino)carbonyl)oxy)propanamide
Leguarme
RN: 16118-49-3 **MP** (°C)**:** >110
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.500E+00	20	M161	1 0 0 0 1	

2880. $C_{12}H_{16}N_2O_3$
Cyclobarbital
Phanodorm
RN: 52-31-3 **MP** (°C)**:** 173
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.772E-03	1.600E+00	20	F300	1 0 0 0 1	
6.941E-03	1.640E+00	20	J030	1 2 2 2 2	
3.500E-02	8.270E+00	25	G003	1 1 1 1 1	pH 4.7
8.000E-03	1.890E+00	30	G014	1 1 1 1 0	EFG
7.800E-03	1.843E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
8.000E-03	1.890E+00	30	K108	1 2 2 0 1	
9.735E-03	2.300E+00	37	F300	1 0 0 0 1	
9.523E-03	2.250E+00	37	J030	1 2 2 2 2	
9.140E-02	2.160E+01	40	N008	1 2 1 1 2	*sic*

2881. $C_{12}H_{16}N_3O_3PS$
Triazophos
O,*O*-Diethyl *O*-(1-phenyl-1H-1,2,4-triazol-3-yl) phosphorothioate
Hostathion
RN: 24017-47-8 **MP** (°C)**:**
MW: 313.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.884E-05	2.470E-02	20	B300	2 1 1 1 2	
1.245E-04	3.900E-02	23	M161	1 0 0 0 1	
1.245E-04	3.900E-02	23	T305	1 0 0 0 1	
1.245E-04	3.899E-02	ns	S460	0 0 0 0 0	

2882. $C_{12}H_{16}N_3O_3PS_2$
Azinphos-ethyl
O,*O*-Diethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
Azinos
Ethyl guthion
RN: 2642-71-9 **MP** (°C)**:**
MW: 345.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B300	2 2 1 1 2	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
7.152E-05	2.470E-02	30	B324	0 0 0 0 0	
7.151E-05	2.470E-02	30	B324	0 0 0 0 0	
3.020E-05	1.043E-02	ns	R427	0 0 0 0 0	

2883. $C_{12}H_{16}N_4O_2$
2,5-Diaziridinyl-3,6-bis(methylamino)-1,4-benzoquinone
Benzoquinone-2,5-bisaziridinyl-3,6-bismethyl amino
RN: 59886-52-1 **MP** (°C)**:** 220
MW: 248.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.03E-04	<1.00E-01	rt	C317	0 0 0 0 0	

2884. $C_{12}H_{16}N_4O_2S_2$
Glybuthiazole
p-Aminobenzenesulfamido-*tert*-butylthiodiazole
Glipasol
Glypasol
RN: 535-65-9 **MP** (°C)**:** 222
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	5.686E-02	37	A046	2 0 1 1 2	

2885. $C_{12}H_{16}N_4O_2S_2$
4-Amino-*N*-(5-butyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Sulfanilamide, *N*1-(5-butyl-1,3,4-thiadiazol-2-yl)-
RN: 71119-31-8 **MP** (°C)**:**
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	8.466E-02	37	A046	2 0 1 1 2	

2886. $C_{12}H_{16}N_4O_7S$
2′-Methylsulfonyl-6-methoxypurine arabinoside
9H-Purine, 6-methoxy-9-[2-*O*-(methylsulfonyl)-β-D-arabinofuranosyl]-
RN: 145913-48-0 **MP** (°C)**:** 188-190
MW: 360.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-02	6.198E+00	37	C348	0 0 0 0 0	pH 7.00

2887. $C_{12}H_{16}N_5O_3PS_2$
Azinphos-ethyl *O*-analog
RN: **MP** (°C)**:**
MW: 373.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-02	3.797E+00	10	B300	2 2 1 1 2	

2888. $C_{12}H_{16}O$
o-Cyclohexylphenol
2-Cyclohexylphenol
RN: 119-42-6 **MP** (°C)**:**
MW: 176.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.727E-04	8.333E-02	25	L021	1 0 0 0 0	

2889. $C_{12}H_{16}O$
p-Cyclohexylphenol
4-Cyclohexylphenol
RN: 1131-60-8 **MP** (°C)**:**
MW: 176.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.782E-04	6.666E-02	25	L021	1 0 0 0 0	

2890. $C_{12}H_{16}O_2$
ε-Phenylcaproic acid
6-Phenylcaproic acid
6-Phenylhexanoic acid
RN: 5581-75-9 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-03	4.798E-01	30	D033	2 2 1 2 2	
4.002E-03	7.694E-01	40	D033	2 2 1 2 2	

2891. $C_{12}H_{16}O_2$
4-Cyclohexylresorcinol
p-Cyclohexylresorcinol
RN: 2138-20-7 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-03	4.998E-01	25	L021	1 0 0 0 0	

2892. $C_{12}H_{16}O_3$
Isoamyl salicylate
Isoamyl *o*-hydroxybenzoate
3-Methylbutyl salicylate
3-Methylbutyl *o*-hydroxybenzoate
RN: 87-20-7 **MP** (°C)**:**
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.961E-04	1.450E-01	25	D081	1 2 2 1 2	
6.918E-04	1.441E-01	ns	S460	0 0 0 0 0	

2893. $C_{12}H_{16}O_7.H_2O$
Arbutin (monohydrate)
Hydroquinone-β-D-glucopyranoside monohydrate
RN: 6058-77-1 **MP** (°C)**:** 195–200
MW: 290.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.828E-01	1.111E+02	c	D004	0 0 0 0 0	
1.723E+00	5.000E+02	h	D004	0 0 0 0 0	

2894. $C_{12}H_{17}NO_2$
2,6-Diethyl-4-acetaminophenol
3,5-Diethylparacetamol
4-Acetamido-2,6-diethylphenol
RN: 55205-89-5 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-03	6.101E-01	25	D078	1 2 1 1 2	

2895. $C_{12}H_{17}NO_2$
Promecarb
5-Isopropyl-*m*-tolyl methylcarbamate
Carbamult
RN: 2631-37-0 **MP** (°C)**:** 87.5
MW: 207.27 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-04	9.200E-02	rt	M161	0 0 0 0 1	

2896. $C_{12}H_{17}NO_2$
Pentyl *p*-aminobenzoate
4-Aminobenzoic acid pentyl ester
RN: 13110-37-7 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	8.084E-02	37	F006	1 1 2 2 1	
1.890E-04	3.917E-02	ns	M066	0 0 0 0 2	
1.890E-04	3.917E-02	rt	B016	0 0 1 1 2	pH 7.4

2897. $C_{12}H_{17}NO_2$
2-*sec*-Butylphenyl methylcarbamate
BPMC
2-(1-Methylpropyl)phenol methylcarbamate
N-Methyl *O*-*sec*-butylphenylcarbamate
RN: 3766-81-2 **MP** (°C)**:** 32
MW: 207.27 **BP** (°C)**:** 112.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.294E-04	8.900E-02	22	K137	1 1 2 1 0	
3.184E-03	6.600E-01	30	M161	1 0 0 0 2	

2898. $C_{12}H_{17}NO_2$
Hexyl nicotinate
n-Hexyl nicotinoate
Nicotinic acid *n*-hexyl ester
RN: 23597-82-2 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.202E-04	1.700E-01	32	L346	1 0 0 1 2	

2899. $C_{12}H_{17}NO_2$
m-tert-Butylphenyl *N*-methylcarbamate
3-*tert*-Butylphenyl *N*-methylcarbamate
RN: 780-11-0 **MP** (°C)**:** 144.0
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.41E-06	<5.00E-04	30	D089	2 2 0 0 0	

2900. $C_{12}H_{17}NO_3$
m-sec-Butoxyphenyl *N*-methylcarbamate
3-*sec*-Butoxyphenyl *N*-methylcarbamate
RN: 13538-22-2 **MP** (°C)**:** 53
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-04	8.000E-02	30	D089	2 2 0 0 0	

2901. $C_{12}H_{17}NO_3$
m-n-Butoxyphenyl *N*-methylcarbamate
3-*n*-Butoxyphenyl *N*-methylcarbamate
RN: 3978-68-5 **MP** (°C)**:** 54.5
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.000E-02	30	D089	2 2 0 0 0	

2902. $C_{12}H_{17}NO_3$
Acetamide, *N*-[4-(1-ethoxyethoxy)phenyl]-
1-(*p*-Acetaminophenoxy)-1-ethoxyethane
RN: 51736-24-4 **MP** (°C)**:**
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.698E-01	ns	H076	0 0 0 0 0	

2903. $C_{12}H_{17}NO_4$
3,5-Dimethoxy-acetophenetide
RN: **MP** (°C)**:**
MW: 239.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.904E-01	1.173E+02	21.80	B102	2 0 1 1 1	solid hydrate
3.344E+00	8.000E+02	35.60	B102	2 0 1 1 2	liquid hydrate
8.778E-01	2.100E+02	39.40	B102	2 0 1 1 1	solid hydrate

(*continued*)

2903. $C_{12}H_{17}NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E+00	7.736E+02	45.60	B102	2 0 1 1 2	liquid hydrate
1.586E+00	3.795E+02	57	B102	2 0 1 1 1	solid hydrate
3.172E+00	7.591E+02	58.10	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	68.50	B102	2 0 1 1 2	liquid hydrate
2.100E+00	5.026E+02	69.50	B102	2 0 1 1 1	solid hydrate
2.288E+00	5.474E+02	72.80	B102	2 0 1 1 1	solid hydrate
2.569E+00	6.147E+02	77.10	B102	2 0 1 1 2	solid hydrate
2.790E+00	6.675E+02	80.20	B102	2 0 1 1 2	solid hydrate
2.947E+00	7.053E+02	82.60	B102	2 0 1 1 2	solid hydrate
3.049E+00	7.296E+02	84.20	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	84.30	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	86	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	86.90	B102	2 0 1 1 2	solid hydrate
3.348E+00	8.011E+02	99.80	B102	2 0 1 1 2	liquid hydrate
3.459E+00	8.275E+02	111.10	B102	2 0 1 1 2	liquid hydrate
3.527E+00	8.440E+02	118.40	B102	2 0 1 1 2	liquid hydrate
3.632E+00	8.690E+02	129.20	B102	2 0 1 1 2	liquid hydrate
4.031E+00	9.645E+02	173.60	B102	2 0 1 1 2	liquid hydrate

2904. $C_{12}H_{17}N_2O_2$

4-Aminobenzoic acid-2-(propyl-amino)ethyl ester
2-(Propylamino)ethyl 4-aminobenzoate
4-Aminobenzoic acid 2-(propyl-amino)ethyl ester

RN: **MP** (°C)**:**
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	6.638E-02	ns	M066	0 0 0 0 0	

2905. $C_{12}H_{17}N_3O_4S$

3′-Nitroso-tolbutamide

RN: **MP** (°C)**:**
MW: 299.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.341E-04	1.000E-01	25	G051	1 0 1 1 0	

2906. $C_{12}H_{17}N_5O_3$

N,*N*-Diethylglycyloxymethyl-1-allopurinol
Glycine, *N*,*N*-diethyl-, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98204-08-1 **MP** (°C)**:**
MW: 279.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-02	4.500E+00	22	B323	0 0 0 0 0	

2907. $C_{12}H_{17}O_4PS_2$
Phenthoate
Dimethyl-*S*-(α-ethoxycarbonylbenzyl) phosphorodithioate
Elsan
Fenthoate
Phent
Cidial
RN: 2597-03-7 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-04	2.000E-01	20	M161	1 0 0 0 2	
3.434E-05	1.100E-02	22	K137	1 1 2 1 0	
3.119E-05	9.992E-03	ns	S460	0 0 0 0 0	

2908. $C_{12}H_{18}$
1-Phenylhexane
Hexylbenzene
n-Hexylbenzene
RN: 1077-16-3 **MP** (°C)**:** –61
MW: 162.28 **BP** (°C)**:** 226

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-06	9.214E-04	5.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	6.04	M183	1 2 1 1 2	
5.140E-06	8.341E-04	7	O312	2 2 0 2 2	
5.667E-06	9.196E-04	8.04	M183	1 2 1 1 2	
5.583E-06	9.060E-04	9.04	M183	1 2 1 1 2	
5.150E-06	8.357E-04	10	O312	2 2 0 2 2	
5.572E-06	9.042E-04	10.04	M183	1 2 1 1 2	
5.717E-06	9.277E-04	11.04	M183	1 2 1 1 2	
5.733E-06	9.304E-04	12.04	M183	1 2 1 1 2	
5.667E-06	9.196E-04	13.04	M183	1 2 1 1 2	
5.700E-06	9.250E-04	14.04	M183	1 2 1 1 2	
5.090E-06	8.260E-04	15	O312	2 2 0 2 2	
5.594E-06	9.079E-04	15.04	M183	1 2 1 1 2	
5.661E-06	9.187E-04	16.04	M183	1 2 1 1 2	
5.606E-06	9.097E-04	17.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	18.04	M183	1 2 1 1 2	
5.811E-06	9.430E-04	19.04	M183	1 2 1 1 2	
5.860E-06	9.509E-04	20	O312	2 2 0 2 2	
5.850E-06	9.493E-04	20.04	M183	1 2 1 1 2	
5.889E-06	9.556E-04	21.04	M183	1 2 1 1 2	
5.872E-06	9.529E-04	22.04	M183	1 2 1 1 2	
6.056E-06	9.827E-04	23.04	M183	1 2 1 1 2	
6.133E-06	9.953E-04	24.04	M183	1 2 1 1 2	
6.270E-06	1.017E-03	25	M342	1 0 1 1 2	
5.560E-06	9.023E-04	25	O312	2 2 0 2 2	

(*continued*)

2908. $C_{12}H_{18}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.156E-06	9.989E-04	25.04	M183	1 2 1 1 2	
6.156E-06	9.989E-04	26.04	M183	1 2 1 1 2	
6.239E-06	1.012E-03	27.04	M183	1 2 1 1 2	
6.261E-06	1.016E-03	29.04	M183	1 2 1 1 2	
6.140E-06	9.964E-04	30	O312	2 2 0 2 2	
6.590E-06	1.069E-03	35	O312	2 2 0 2 2	
6.590E-06	1.069E-03	40	O312	2 2 0 2 2	
8.000E-06	1.298E-03	45	O312	2 2 0 2 2	
2.000E-03	3.246E-01	ns	H307	0 0 0 0 0	

2909. $C_{12}H_{18}N_2O$

Isoproturon
N,*N*-Dimethyl-*N′*-(4-(1-methylethyl)phenyl)urea
3-(4-Isopropylphenyl)-1,1-dimethylurea
Tolkan
DPX 6774

RN: 34123-59-6 **MP** (°C)**:** 158.5
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.909E-04	6.000E-02	20	M161	1 0 0 0 1	

2910. $C_{12}H_{18}N_2O_2$

Zectran
4-Dimethylamino-3,5-dimethylphenol methylcarbamate ester
Mexacarbole
Mexacarbate

RN: 315-18-4 **MP** (°C)**:** 85
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E-04	9.999E-02	25	I314	0 0 0 0 0	

2911. $C_{12}H_{18}N_2O_2S$

Thiamylal
5-Allyl-5-(1-methyl-butyl)-barbituric acid
5-Allyl-5-(1-methylbutyl)-2-thiobarbituric acid

RN: 77-27-0 **MP** (°C)**:** 132
MW: 254.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.104E-03	1.298E+00	25	A023	1 0 0 1 1	
1.966E-04	5.000E-02	25	B011	2 0 0 1 0	
1.944E-04	4.946E-02	25	B065	1 1 1 1 2	

(*continued*)

2911. $C_{12}H_{18}N_2O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-04	8.852E-02	25	G003	1 1 1 1 1	pH 4.7
7.500E-03	1.908E+00	30	G014	1 1 1 1 0	EFG
6.600E-03	1.679E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
8.630E-03	2.195E+00	40	A023	1 0 0 1 1	
3.750E-03	9.538E-01	40	N008	1 2 1 1 2	*sic*
8.792E-03	2.236E+00	ns	G039	0 0 0 0 0	EFG

2912. $C_{12}H_{18}N_2O_3$

5-Isopropyl-5-(3-methylbut-2-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methyl-2-butenyl)-5-(1-methylethyl)
5-*i*-Propyl-5-(3-methylbut-2-enyl)barbiturate

RN: 67051-26-7 **MP** (°C)**:**
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-03	6.088E-01	25	P350	0 0 0 0 0	intrinsic

2913. $C_{12}H_{18}N_2O_3$

Secobarbital
5-Allyl-5-(1-methylbutyl)barbituric acid
Seconal

RN: 76-73-3 **MP** (°C)**:** 98
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.250E-03	1.728E+00	25	G003	1 1 1 1 2	pH 7
4.410E-03	1.051E+00	25	V033	2 0 1 1 2	
4.400E-03	1.048E+00	25.00	T303	1 0 0 0 1	
6.300E-03	1.501E+00	35.00	T303	1 0 0 0 1	
7.900E-02	1.882E+01	40	N008	1 0 1 1 2	*sic*
9.400E-03	2.240E+00	45.00	T303	1 0 0 0 1	

2914. $C_{12}H_{18}N_2O_3S$

Tolbutamide
1-Butyl-3-(*para*-tolylsulfonyl) urea
Oramide
Orinase

RN: 64-77-7 **MP** (°C)**:** 129
MW: 270.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.178E-04	1.400E-01	25	G051	1 0 1 1 0	
4.068E-04	1.100E-01	25	P096	0 0 0 0 0	

(*continued*)

2914. $C_{12}H_{18}N_2O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.054E-01	30	G318	0 0 0 0 0	EFG
4.027E-04	1.089E-01	37	A028	1 0 2 1 2	intrinsic
4.030E-04	1.090E-01	37	A046	2 0 1 1 2	
5.659E-04	1.530E-01	37	B138	1 2 0 0 2	pH 1.5, form II
5.289E-04	1.430E-01	37	B138	1 2 0 0 2	pH 1.5, form III
5.067E-04	1.370E-01	37	B138	1 2 0 0 2	pH 1.5, form I
3.699E-04	1.000E-01	37.0	H033	1 0 2 1 0	pH 1.4, intrinsic
3.031E-03	8.193E-01	37.5	F015	1 0 2 2 1	pH 6.0, pKa 5.32
2.535E-02	6.853E+00	37.5	F015	1 0 2 2 2	pH 7.0, pKa 5.32

2915. $C_{12}H_{18}N_2O_4S$

Anisylbutamide
Methoxyphenylbutazolamide
Methoxytolbutamide

RN: 24535-67-9 **MP** (°C)**:**
MW: 286.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.236E-04	1.213E-01	37	A028	1 0 2 1 2	intrinsic
4.260E-04	1.220E-01	37	A046	2 0 1 1 2	

2916. $C_{12}H_{18}N_2O_5$

D-Mannosephenylhydrazone
D-Mannose-phenylhydrazon

RN: 6147-14-4 **MP** (°C)**:** 195.5
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.811E-02	1.030E+01	100	F300	1 0 0 0 2	

2917. $C_{12}H_{18}N_4O_6S$

Oryzalin
3,5-Dinitro-*N*4,*N*4-dipropylsulfanilamide

RN: 19044-88-3 **MP** (°C)**:** 137
MW: 346.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-04	8.500E-02	25	B200	1 0 0 0 1	
6.929E-06	2.400E-03	25	M161	1 0 0 0 1	

2918. $C_{12}H_{18}O$
Propofol
2,6-Diisopropylphenol
Diisopropylphenol
Diprivan
RN: 2078-54-8 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.975E-04	1.600E-01	amb	L434	0 0 0 0 0	

2919. $C_{12}H_{18}O$
2-Butyl-4-ethylphenol
Phenol, 2-butyl-4-ethyl-
RN: 3781-74-6 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2920. $C_{12}H_{18}O$
2-Butyl-4,6-dimethylphenol
2,6-Xylenol, 2-butyl-
RN: 6483-60-9 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L020	1 0 0 0 0	

2921. $C_{12}H_{18}O$
o-*n*-Hexylphenol
2-*n*-Hexylphenol
RN: 3226-32-2 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L022	1 0 0 0 0	

2922. $C_{12}H_{18}O$
2-Butyl-4,5-dimethylphenol
Phenol, 2-butyl-4,5-dimethyl-
RN: **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2923. $C_{12}H_{18}O$
2-Butyl-6-ethylphenol
Phenol, 2-butyl-6-ethyl-
RN: 22496-45-3 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2924. $C_{12}H_{18}O$
2,6-Dipropylphenol
Phenol, 2,6-dipropyl-
RN: 6626-32-0 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2925. $C_{12}H_{18}O$
4-Butyl-2,5-dimethylphenol
2,5-Xylenol, 4-butyl-
RN: 91763-77-8 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2926. $C_{12}H_{18}O$
4-Butyl-2,6-dimethylphenol
Phenol, 4-butyl-2,6-dimethyl-
2,6-Xylenol, 4-butyl-
RN: 6676-26-2 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2927. $C_{12}H_{18}O$
p-*n*-Hexylphenol
4-*n*-Hexylphenol
RN: 2446-69-7 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L022	1 0 0 0 0	

2928. $C_{12}H_{18}O$
2,4-Dipropylphenol
Phenol, 2,4-dipropyl-
RN: 23167-99-9 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2929. $C_{12}H_{18}O_2$
4-Hexylresorcinol
4-*n*-Hexylresorcin
RN: 136-77-6 **MP** (°C)**:** 68
MW: 194.28 **BP** (°C)**:** 334

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.574E-03	5.000E-01	18	F300	1 0 0 0 1	

2930. $C_{12}H_{18}O_4S_2$
Di-isopropyl 1,3-dithiolan-2-ylidinemalonate
Isoprothiolane
Fuji-one
bis(1-Methylethyl) 1,3-dithiolan-2-ylidenepropanedioate
RN: 50512-35-1 **MP** (°C)**:** 52.25
MW: 290.40 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	4.800E-02	20	H309	0 0 0 0 0	
1.653E-04	4.800E-02	20	M161	1 0 0 0 1	

2931. $C_{12}H_{19}BrN_2O_2$
Neostigmine bromide
Neostigmine bromide
Neostigmine;
Prostigmin
RN: 114-80-7 **MP** (°C)**:**
MW: 303.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.298E+00	1.000E+03	ns	K444	0 0 0 0 0	

2932. $C_{12}H_{19}ClNO_3P$
Crufomate
O-Methyl *O*-2-chloro-4-*tert*-butyphenyl *N*-methylamidophosphate
RN: 299-86-5 **MP** (°C)**:** 60.25
MW: 291.72 **BP** (°C)**:** 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-02	4.975E+00	ns	M061	0 0 0 0 0	

2933. $C_{12}H_{19}N_3O_8$
Orotic acid methylglucamide
RN: **MP** (°C)**:** 184–186
MW: 333.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-01	1.490E+02	–4	N018	0 0 0 0 0	
7.090E-01	2.363E+02	16	N018	0 0 0 0 0	
8.150E-01	2.716E+02	25	N018	0 0 0 0 0	

2934. $C_{12}H_{19}N_6OP$
Triamiphos
5-Amino-1-(bis(dimethylamino)phosphoryl)-3-phenyl-1,2,4-triazole
Triamifos
Wepsyn 155
Wepsyn
bis(Dimethylamino)-(3-amino-5-phenyl-1,2,4-triazol-1-yl)-phosphine oxide
RN: 1031-47-6 **MP** (°C)**:** 167.5
MW: 294.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.495E-04	2.500E-01	20	M161	1 0 0 0 2	

2935. $C_{12}H_{19}O_2PS_3$
Sulprofos
O-Ethyl *O*-[4-(methylthio)phenyl]phosphorodithioic acid *S*-propyl ester
Morpafos
Bolstar
Heliothion
Merdafos
RN: 35400-43-2 **MP** (°C)**:**
MW: 322.45 **BP** (°C)**:** 155–158

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.616E-07	3.101E-04	ns	S460	0 0 0 0 0	

2936. $C_{12}H_{20}$
Triisobutene
1,8-Nonadiene, 2,8-dimethyl-5-methylene-
RN: 36370-80-6 **MP** (°C)**:**
MW: 164.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.944E-08	8.123E-06	20	B165	1 0 1 1 1	
5.838E-03	9.591E-01	97.30	B165	1 0 1 1 1	

2937. $C_{12}H_{20}N_2O_3$
5-Ethyl-5-*n*-hexylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-hexyl-
Hexethal
Ortal
Ortol
RN: 77-30-5 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.930E-04	2.146E-01	25	M310	2 2 2 2 2	

2938. $C_{12}H_{20}N_4O_2$
3-Cyclohexyl-6-dimethylamino-1-methyl-1,3,5-triazine-2,4-dione
1,3,5-Triazine-2,4(1H,3H)-dione, 3-cyclohexyl-6-(dimethylamino)-1-methyl-
Hexazinone
Pronone
DPX 3674
RN: 51235-04-2 **MP** (°C)**:** 116
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.308E-01	3.300E+01	25	M161	1 0 0 0 1	

2939. $C_{12}H_{20}N_4O_6$
Acetyltetraglycine ethyl ester
Glycine, *N*-acetylglycylglycylglycyl-, ethyl ester
RN: 637-83-2 **MP** (°C)**:** 264
MW: 316.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-04	2.600E-01	0	R036	0 0 0 0 0	
2.466E-03	7.800E-01	25	R036	0 0 0 0 0	
5.216E-03	1.650E+00	40	R036	0 0 0 0 0	

2940. $C_{12}H_{20}O_2$
Linalyl acetate
Bergamol
3,7-Dimethyl-1,6-octadien-3-yl acetate
Linalyl
RN: 115-95-7 **MP** (°C)**:**
MW: 196.29 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.546E-03	4.998E-01	25	M350	1 0 1 1 1	

2941. $C_{12}H_{20}O_4$
Dibutyl maleate
Di-*n*-butyl maleate
RN: 105-76-0 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.073E-03	2.450E-01	25	F067	1 0 2 2 2	

2942. $C_{12}H_{20}O_6$
Tripropionin
1,2,3-Propanetriol, tripropanoate
1,2,3-Propanetriyl tripropionate
Tripropionylglycerol
Tripropanoylglycerol
RN: 139-45-7 **MP** (°C)**:**
MW: 260.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-02	3.120E+00	ns	F014	0 0 0 0 2	

2943. $C_{12}H_{21}NO_8S$
Topiramate
2,3:4,5-di-*O*-isopropylidene-β-D-fructopyranose sulfamate
Topamax
Tracrium
RN: 97240-79-4 **MP** (°C)**:**
MW: 339.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-02	9.705E+00	ns	S469	0 0 0 0 0	

2944. $C_{12}H_{21}N_2O_3PS$

Diazinon
O,*O*-Diethyl *O*-(2-isopropyl-6-methyl-4-pyrimidinyl), phosphorothioate
Dimpylate
Basudin
Spectracide
Fezudin

RN: 333-41-5 **MP** (°C)**:** >120
MW: 304.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.336E-04	7.109E-02	10	B324	0 0 0 0 0	
2.336E-04	7.110E-02	10	B324	0 0 0 0 0	
1.318E-04	4.012E-02	20	B179	0 0 0 0 0	
2.261E-04	6.881E-02	20	B300	2 1 1 1 2	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.314E-04	4.000E-02	20	M061	1 0 0 0 1	
2.260E-04	6.880E-02	22	B169	2 1 1 1 2	
1.331E-04	4.050E-02	22	K137	1 1 2 1 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.314E-04	4.000E-02	rt	M161	0 0 0 0 1	

2945. $C_{12}H_{21}N_5O_2S_2$

Nizatidine
Axid
N-(2-(((2-((Dimethylamino)methyl)-4-thiazolyl)methyl)thio)ethyl)-*N′*-methyl-2-nitro-1,1-ethenediamine

RN: 76963-41-2 **MP** (°C)**:**
MW: 331.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.457E-02	2.140E+01	ns	R427	0 0 0 0 0	

2946. $C_{12}H_{21}N_7O$

1-(4′-Formyl-1-piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine
1-Piperazinecarboxaldehyde, 4-[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]-

RN: 126974-79-6 **MP** (°C)**:**
MW: 279.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.670E-03	1.025E+00	25	B386	0 0 0 0 0	

2947. $C_{12}H_{22}N_2O_2$
N,*N*,*N*′,*N*′-Tetraethylfumaramide
2-Butenediamide, *N*,*N*,*N*′,*N*′-tetraethyl-
RN: 111328-65-5 **MP** (°C)**:**
MW: 226.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	1.562E+02	30	K019	1 0 0 0 1	

2948. $C_{12}H_{22}N_6$
1-(Piperidinyl)-3,5-bis(dimethylamino)-*s*-triazine
s-Triazine, 2,4-bis(dimethylamino)-6-piperidino-
RN: 16268-79-4 **MP** (°C)**:**
MW: 250.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	4.402E-02	25	B386	0 0 0 0 0	

2949. $C_{12}H_{22}O_2$
Arbanol
RN: 7070-15-7 **MP** (°C)**:**
MW: 198.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	3.020E-01	6	P430	0 0 0 0 0	
2.911E-03	5.773E-01	23.5	P430	0 0 0 0 0	

2950. $C_{12}H_{22}O_4$
Ethylene glycol divalerate
RN: **MP** (°C)**:**
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.460E-04	1.488E-01	25	F064	1 0 0 0 2	

2951. $C_{12}H_{22}O_4$
1,10-Decanedicarboxylic acid
Decan-dicarbonsaeure-(1,10)
Dodecanedioc acid
RN: 693-23-2 **MP** (°C)**:** 128
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	4.000E-02	20	F300	1 0 0 0 0	
3.039E-03	7.000E-01	21	B040	1 0 1 1 0	*sic*
5.124E-03	1.180E+00	100	F300	1 0 0 0 2	

2952. $C_{12}H_{22}O_4$
Dibutyl succinate
Succinic acid di-*n*-butyl ester
Tabutrex
RN: 141-03-7 **MP** (°C)**:** –29
MW: 230.31 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.984E-04	2.299E-01	ns	F014	0 0 0 0 1	

2953. $C_{12}H_{22}O_6$
Triethylene glycol dipropionate
Ethanol, 2,2′-[1,2-ethanediylbis(oxy)]*bis*-, dipropanoate
RN: 141-34-4 **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.394E-01	6.279E+01	ns	F014	0 0 0 0 2	

2954. $C_{12}H_{22}O_6$
Dibutyl tartrate
(2R,3R)-Di-*n*-butyl tartrate
ENT 396
RN: 87-92-3 **MP** (°C)**:** 21
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.840E-02	4.827E+00	ns	F014	0 0 0 0 2	

2955. $C_{12}H_{22}O_6$
Dimethoxyethyl adipate
RN: **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.338E-02	1.400E+01	ns	F014	0 0 0 0 2	

2956. $C_{12}H_{22}O_{11}$
Maltose
D-Glucose, 4-*O*-α-D-glucopyranosyl-
α-Maltose
Malt sugar
RN: 69-79-4 **MP** (°C)**:** 102.5
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.166E-01	2.453E+02	0	C401	1 0 0 0 0	EFG
1.061E+00	3.631E+02	0	M043	1 0 0 0 1	
1.151E+00	3.939E+02	10	M043	1 0 0 0 1	
9.066E-01	3.103E+02	20	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	20	D041	1 0 0 0 2	
1.280E+00	4.382E+02	20	M043	1 0 0 0 1	
1.408E+00	4.819E+02	30	M043	1 0 0 0 1	
1.124E+00	3.846E+02	40	C401	1 0 0 0 0	EFG
1.037E+00	3.548E+02	40	C401	1 0 0 0 0	EFG
1.530E+00	5.238E+02	40	M043	1 0 0 0 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.859E+00	6.364E+02	60	M043	1 0 0 0 2	
1.298E+00	4.444E+02	80	C401	1 0 0 0 0	EFG
2.191E+00	7.500E+02	80	M043	1 0 0 0 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	rt	D021	0 0 1 1 2	

2957. $C_{12}H_{22}O_{11}$
β-Lactose
B-Lactose
Milchzucker
4-*O*-β-D-Galactopyranosyl-D-glucose
RN: 5965-66-2 **MP** (°C)**:** 253
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.525E-01	5.220E+01	20	F300	1 0 0 0 2	
7.303E-02	2.500E+01	h	F300	0 0 0 0 1	

2958. $C_{12}H_{22}O_{11}$
Cellobiose
4-*O*-β-D-Glucopyranosyl-D-glucose
4-β-D-Glucopyransoyl-D-glucopyranose
D-(+)-Cellobiose
RN: 528-50-7 **MP** (°C)**:**
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.243E-01	1.110E+02	15	F300	1 0 0 0 2	
3.475E-01	1.189E+02	30.50	M137	2 1 2 2 2	
1.198E+00	4.100E+02	h	F300	0 0 0 0 1	

2959. $C_{12}H_{22}O_{11}$
Lactose
4-*O*-B-D-Galactopyranosyl-D-glucose
Milk sugar
RN: 63-42-3 **MP** (°C)**:** 201
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.656E-01	9.091E+01	0	C401	1 0 0 0 0	EFG
3.177E-01	1.087E+02	0	M043	1 0 0 0 2	
3.116E-01	1.067E+02	0	P052	1 0 2 2 2	
4.701E-01	1.609E+02	1	P049	1 0 1 1 1	
3.811E-01	1.304E+02	10	M043	1 0 0 0 2	
4.351E-01	1.489E+02	20	C401	1 0 0 0 0	EFG
4.767E-01	1.632E+02	20	M043	1 0 0 0 2	
5.189E-01	1.776E+02	25	D041	1 0 0 0 2	
5.470E-01	1.873E+02	25	P049	1 0 1 1 1	
6.000E-01	2.054E+02	30	D011	1 0 1 0 1	
5.880E-01	2.013E+02	30	M043	1 0 0 0 2	
5.843E-01	2.000E+02	40	C401	1 0 0 0 0	EFG
7.298E-01	2.498E+02	40	M043	1 0 0 0 2	
7.574E-01	2.593E+02	60	C401	1 0 0 0 0	EFG
1.067E+00	3.651E+02	60	M043	1 0 0 0 2	
9.738E-01	3.333E+02	80	C401	1 0 0 0 0	EFG
1.475E+00	5.050E+02	80	M043	1 0 0 0 2	
1.699E+00	5.816E+02	89	D041	1 0 0 0 2	
1.096E+00	3.750E+02	95	C401	1 0 0 0 0	EFG
1.124E+00	3.846E+02	100	C401	1 0 0 0 0	EFG
1.767E+00	6.047E+02	100	M043	1 0 0 0 2	
4.775E-01	1.635E+02	rt	D021	0 0 1 1 2	

2960. $C_{12}H_{22}O_{11}$
Sucrose
Saccharose
β-D-Fructofuranosyl-α-D-glucopyranoside
α-D-Glucopyranosyl β-D-fructofuranoside
Beet sugar
Cane sugar
RN: 57-50-1 **MP** (°C)**:** 191
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E+00	3.902E+02	0	C401	1 0 0 0 0	EFG
1.878E+00	6.429E+02	0	D041	1 0 0 0 2	
1.876E+00	6.421E+02	0	G046	1 0 1 1 2	
1.142E+00	3.909E+02	0	H094	1 0 0 0 2	
1.874E+00	6.416E+02	0	M043	1 0 0 0 2	
1.884E+00	6.450E+02	0	P052	1 0 2 2 2	
1.880E+00	6.435E+02	.90	M074	1 0 0 0 2	average of 3
1.157E+00	3.961E+02	10	H094	1 0 0 0 2	
1.914E+00	6.552E+02	10	M043	1 0 0 0 2	
1.943E+00	6.650E+02	12.5	F300	1 0 0 0 2	
1.938E+00	6.633E+02	15	D041	1 0 0 0 2	
1.934E+00	6.622E+02	15.80	M074	1 0 0 0 2	average of 3
1.931E+00	6.609E+02	18.5	W013	1 2 1 1 2	
1.177E+00	4.030E+02	20	C401	1 0 0 0 0	EFG
1.203E+00	4.118E+02	20	C401	1 0 0 0 0	EFG
1.946E+00	6.660E+02	20	F300	1 0 0 0 2	
1.170E+00	4.005E+02	20	G060	1 0 0 0 2	
1.173E+00	4.015E+02	20	H094	1 0 0 0 2	
1.960E+00	6.711E+02	20	M043	1 0 0 0 2	
1.956E+00	6.697E+02	23.9	W013	1 2 1 1 2	
1.954E+00	6.689E+02	24.4	W013	1 2 1 1 2	
1.964E+00	6.723E+02	24.9	W013	1 2 1 1 2	
1.986E+00	6.798E+02	25	G046	1 0 1 1 2	
1.179E+00	4.036E+02	25	G060	1 0 0 0 2	
1.981E+00	6.779E+02	25.60	M074	1 0 0 0 2	average of 3
1.963E+00	6.721E+02	25.9	W013	1 2 1 1 2	
1.188E+00	4.067E+02	30	G060	1 0 0 0 2	
1.190E+00	4.072E+02	30	H094	1 0 0 0 2	
2.006E+00	6.865E+02	30	M043	1 0 0 0 2	
1.997E+00	6.836E+02	30.0	W013	1 2 1 1 2	
1.996E+00	6.831E+02	30.5	W013	1 2 1 1 2	
2.003E+00	6.855E+02	30.50	M074	1 0 0 0 2	average of 3
2.008E+00	6.873E+02	31.5	W013	1 2 1 1 2	
2.005E+00	6.862E+02	33.1	W013	1 2 1 1 2	
2.025E+00	6.932E+02	34.5	W013	1 2 1 1 2	
2.030E+00	6.950E+02	35	G046	1 0 1 1 2	
1.198E+00	4.100E+02	35	G060	1 0 0 0 2	
2.028E+00	6.942E+02	36.0	W013	1 2 1 1 2	
2.028E+00	6.941E+02	36.4	W013	1 2 1 1 2	
1.252E+00	4.286E+02	40	C401	1 0 0 0 0	EFG

(*continued*)

2960. $C_{12}H_{22}O_{11}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E+00	4.133E+02	40	G060	1 0 0 0 2	
1.207E+00	4.132E+02	40	H094	1 0 0 0 2	
2.057E+00	7.041E+02	40	M043	1 0 0 0 2	
2.050E+00	7.017E+02	40.2	W013	1 2 1 1 2	
2.052E+00	7.023E+02	40.7	W013	1 2 1 1 2	
2.055E+00	7.035E+02	41.0	W013	1 2 1 1 2	
2.061E+00	7.055E+02	42.2	W013	1 2 1 1 2	
2.067E+00	7.074E+02	42.3	W013	1 2 1 1 2	
2.080E+00	7.120E+02	45	F300	1 0 0 0 2	
1.217E+00	4.167E+02	45	G060	1 0 0 0 2	
2.093E+00	7.163E+02	46.1	W013	1 2 1 1 2	
2.107E+00	7.212E+02	49.6	W013	1 2 1 1 2	
2.111E+00	7.225E+02	50	G046	1 0 1 1 2	
1.228E+00	4.202E+02	50	G060	1 0 0 0 2	
7.596E+00	2.600E+03	50	H063	1 0 0 0 2	
1.225E+00	4.194E+02	50	H094	1 0 0 0 2	
2.101E+00	7.191E+02	50.2	W013	1 2 1 1 2	
2.118E+00	7.251E+02	51.1	W013	1 2 1 1 2	
2.124E+00	7.272E+02	52.2	W013	1 2 1 1 2	
2.126E+00	7.276E+02	52.6	W013	1 2 1 1 2	
2.134E+00	7.304E+02	53.6	W013	1 2 1 1 2	
2.134E+00	7.305E+02	53.8	W013	1 2 1 1 2	
2.126E+00	7.278E+02	54.1	W013	1 2 1 1 2	
1.237E+00	4.235E+02	55	G060	1 0 0 0 2	
2.137E+00	7.316E+02	55.8	W013	1 2 1 1 2	
2.147E+00	7.350E+02	56.1	W013	1 2 1 1 2	
2.154E+00	7.372E+02	56.4	W013	1 2 1 1 2	
2.151E+00	7.364E+02	57.5	W013	1 2 1 1 2	
2.154E+00	7.374E+02	57.8	W013	1 2 1 1 2	
2.152E+00	7.368E+02	58.4	W013	1 2 1 1 2	
2.165E+00	7.410E+02	58.6	W013	1 2 1 1 2	
2.166E+00	7.415E+02	59.7	W013	1 2 1 1 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.248E+00	4.273E+02	60	G060	1 0 0 0 2	
1.244E+00	4.259E+02	60	H094	1 0 0 0 2	
2.167E+00	7.416E+02	60	M043	1 0 0 0 2	
2.176E+00	7.448E+02	61.1	W013	1 2 1 1 2	
2.176E+00	7.447E+02	61.4	W013	1 2 1 1 2	
2.182E+00	7.469E+02	62.6	W013	1 2 1 1 2	
2.189E+00	7.493E+02	62.9	W013	1 2 1 1 2	
2.193E+00	7.505E+02	64.6	W013	1 2 1 1 2	
1.258E+00	4.307E+02	65	G060	1 0 0 0 2	
2.204E+00	7.543E+02	65.5	W013	1 2 1 1 2	
2.214E+00	7.580E+02	66.4	W013	1 2 1 1 2	
2.219E+00	7.595E+02	66.5	W013	1 2 1 1 2	
2.222E+00	7.607E+02	68.2	W013	1 2 1 1 2	
2.221E+00	7.603E+02	69.0	W013	1 2 1 1 2	
1.269E+00	4.344E+02	70	G060	1 0 0 0 2	

(*continued*)

2960. $C_{12}H_{22}O_{11}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E+00	7.632E+02	70.1	W013	1 2 1 1 2	
2.233E+00	7.645E+02	70.4	W013	1 2 1 1 2	
2.251E+00	7.706E+02	72.8	W013	1 2 1 1 2	
2.249E+00	7.698E+02	73.8	W013	1 2 1 1 2	
2.267E+00	7.760E+02	74.5	W013	1 2 1 1 2	
2.265E+00	7.752E+02	74.6	W013	1 2 1 1 2	
2.256E+00	7.724E+02	75	G046	1 0 1 1 2	
1.280E+00	4.380E+02	75	G060	1 0 0 0 2	
2.266E+00	7.758E+02	75.1	W013	1 2 1 1 2	
2.290E+00	7.840E+02	79.5	W013	1 2 1 1 2	
1.276E+00	4.366E+02	80	C401	1 0 0 0 0	EFG
1.291E+00	4.417E+02	80	G060	1 0 0 0 2	
1.090E+01	3.730E+03	80	H063	1 0 0 0 2	
2.289E+00	7.835E+02	80	M043	1 0 0 0 2	
2.304E+00	7.886E+02	82.3	W013	1 2 1 1 2	
2.333E+00	7.985E+02	85.1	W013	1 2 1 1 2	
2.335E+00	7.994E+02	85.3	W013	1 2 1 1 2	
2.337E+00	7.999E+02	85.5	W013	1 2 1 1 2	
2.344E+00	8.022E+02	86.6	W013	1 2 1 1 2	
2.346E+00	8.032E+02	88.0	W013	1 2 1 1 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
2.355E+00	8.061E+02	90	G046	1 0 1 1 2	
2.363E+00	8.087E+02	90.2	W013	1 2 1 1 2	
2.388E+00	8.176E+02	95	G046	1 0 1 1 2	
2.409E+00	8.247E+02	98	G046	1 0 1 1 2	
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
2.424E+00	8.296E+02	100	D041	1 0 0 0 2	
2.424E+00	8.296E+02	100	G046	1 0 1 1 2	
2.424E+00	8.296E+02	100	M043	1 0 0 0 2	

2961. $C_{12}H_{23}NO_3$

Propylbutylaceturethane

RN: **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E-03	3.199E-01	20	O021	1 2 0 0 0	

2962. $C_{12}H_{23}N_7$

1-(4′-Methyl-1-piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine

2-(4-Methyl-1-piperazinyl)-4,6-bis(dimethylamino)-*s*-triazine

RN: 5512-05-0 **MP** (°C)**:**

MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.514E-03	1.198E+00	25	B386	0 0 0 0 0	

2963. $C_{12}H_{24}N_2O_2$
N,*N*,*N*′,*N*′-Tetramethylsuberamide
Octanediamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 27397-05-3 **MP** (°C)**:**
MW: 228.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	5.754E+02	30	D010	1 2 1 1 2	

2964. $C_{12}H_{24}N_3O_3PS$
Thiophosphoryl trimorpholide
Morpholine, 4,4′,4″-phosphinothioylidynetris-
Phosphine sulfide, trimorpholino-
RN: 14129-98-7 **MP** (°C)**:**
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.987E-03	3.210E+00	25	A040	1 0 0 0 2	

2965. $C_{12}H_{24}N_3O_4P$
Phosphoryl trimorpholide
Morpholine, 4,4′,4″-phosphinylidynetris-
Phosphine oxide, trimorpholino-
RN: 4441-12-7 **MP** (°C)**:**
MW: 305.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E+00	6.072E+02	25	A040	1 0 0 0 2	

2966. $C_{12}H_{24}N_6$
*N*2,*N*4,*N*6-Triethyl-*N*2,*N*4,*N*6-trimethylmelamine
1,3,5-Triazine-2,4,6-triamine, *N*,*N*′,*N*″-triethyl-*N*,*N*′,*N*″-trimethyl-
RN: 64124-20-5 **MP** (°C)**:**
MW: 252.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-04	5.000E-02	25	C051	1 2 1 1 0	pH 7

2967. $C_{12}H_{24}N_9P_3$
Hexaziridinocyclotriphosphazene
2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis(1-aziridinyl)-1,3,5,2,4,6-triazatriphosphorine
2,2,4,4,6,6-Hexakis(1-aziridinyl)cyclotriphosphaza-1,3,5-triene
Apholate
APN
ENT 26316
RN: 52-46-0 **MP** (°C)**:**
MW: 387.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-01	1.000E+02	ns	L076	0 1 0 0 0	approximate

2968. $C_{12}H_{24}O_2$
Lauric acid
Dodecanoic acid
Laurostearic acid
RN: 143-07-7 **MP** (°C)**:** 44
MW: 200.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.847E-04	3.700E-02	0	B136	1 0 2 1 1	
2.895E-04	5.800E-02	20	B136	1 0 2 1 1	
2.745E-04	5.500E-02	20	D041	1 0 0 0 1	
2.745E-04	5.500E-02	20.0	R001	1 1 1 1 1	
2.400E-05	4.808E-03	25	J001	1 0 2 1 2	
8.486E-06	1.700E-03	25	M083	1 0 0 1 1	
1.150E-05	2.304E-03	25	R002	0 0 0 0 0	intrinsic
2.080E-05	4.167E-03	25	R002	0 0 0 0 0	
3.345E-04	6.700E-02	30	B136	1 0 2 1 1	
3.145E-04	6.300E-02	30.0	R001	1 1 1 1 1	
3.494E-04	7.000E-02	40	B136	1 0 2 1 1	
3.844E-05	7.700E-03	40	E005	2 1 1 2 1	
3.744E-04	7.500E-02	45	B136	1 0 2 1 1	
3.744E-04	7.499E-02	45.0	R001	1 1 1 1 1	
4.593E-05	9.200E-03	50	E005	2 1 1 2 1	
5.470E-05	1.096E-02	50	J001	1 0 2 1 2	
4.343E-04	8.700E-02	60	B136	1 0 2 1 1	
5.791E-05	1.160E-02	60	E005	2 1 1 2 2	
4.343E-04	8.699E-02	60.0	R001	1 1 1 1 1	
1.847E-04	3.700E-02	.0	R001	1 1 1 1 1	

2969. $C_{12}H_{24}O_2$
3-Hydroxy-2,2,5,5-tetraethyltetrahydrofuran
3-Furanol, 2,2,5,5-tetraethyltetrahydro-
RN: 29839-78-9 **MP** (°C)**:**
MW: 200.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.493E-02	2.991E+00	rt	B066	0 2 0 0 0	

2970. $C_{12}H_{24}O_3$
1,3-Dioxolane-4-methanol, 2-heptyl-2-methyl
2-Heptyl-4-hydroxymethyl-2-methyl-1,3-dioxolane
RN: 5660-50-4 **MP** (°C)**:**
MW: 216.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-03	7.701E-01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2971. $C_{12}H_{24}O_4$
1,3-Dioxolane-4-methanol, 2-methyl-2-[2-(pentyloxy)ethyl]
RN: 143458-56-4 **MP** (°C)**:**
MW: 232.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.250E-02	1.452E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2972. $C_{12}H_{26}$
2-Methylundecane
Isododecane
RN: 31807-55-3 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E-08	2.000E-06	25	T423	0 0 0 0 0	

2973. $C_{12}H_{26}$
3,3,6,6-Tetramethyloctane
RN: 62199-46-6 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-07	2.100E-05	25	T423	0 0 0 0 0	

2974. $C_{12}H_{26}$
Dodecane
N-Dodecane
Alkane C(12)
Duodecane
Bihexyl
Adakane 12
RN: 112-40-3 **MP** (°C)**:** –9.6
MW: 170.34 **BP** (°C)**:** 216.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.931E-08	8.400E-06	22.5	G301	0 0 0 0 0	
2.055E-08	3.500E-06	23	C332	0 0 0 0 0	
1.068E-08	1.820E-06	25	B156	1 0 2 2 2	
4.944E-08	8.422E-06	25	F004	0 0 0 0 0	
5.871E-09	1.000E-06	25	T423	0 0 0 0 0	
3.900E-09	6.643E-07	ns	D348	0 0 0 0 0	
2.231E-08	3.800E-06	ns	H123	0 0 0 0 0	

2975. $C_{12}H_{26}$
2,2,4,6,6-Pentamethylheptane
RN: 13475-82-6 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	2.500E-05	25	T423	0 0 0 0 0	

2976. $C_{12}H_{26}O$
Dodecanol
Dodecyl alcohol
Lauryl alcohol
Undecyl carbinol
RN: 112-53-8 **MP** (°C)**:** 24
MW: 186.34 **BP** (°C)**:** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-06	1.696E-03	16	K011	1 2 1 1 2	
2.300E-05	4.286E-03	25	R002	0 0 0 0 0	
1.560E-05	2.907E-03	34	K011	1 2 1 1 2	
1.930E-05	3.596E-03	49	K011	1 2 1 1 2	

2977. $C_{12}H_{27}N$
Tributylamine
tris-n-Butylamine
N,*N*-Dibutyl-1-butanamine
RN: 102-82-9 **MP** (°C)**:** –70
MW: 185.36 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.649E-04	1.418E-01	25.04	V013	2 2 2 2 2	

2978. $C_{12}H_{27}N.4H_2O$
Dodecylamine (tetrahydrate)
RN: 124-22-1 **MP** (°C)**:**
MW: 257.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.776E-03	7.145E-01	ns	R037	0 2 2 1 0	

2979. $C_{12}H_{27}OP$
Tributyl phosphine oxide
Tributylphosphine oxide
TBPO
RN: 814-29-9 **MP** (°C)**:** 64
MW: 218.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E+00	2.260E+02	13.20	H031	1 2 2 2 2	
8.794E-01	1.920E+02	13.40	H031	1 2 2 2 2	
4.718E-01	1.030E+02	16.30	H031	1 2 2 2 2	
1.832E-01	4.000E+01	25	B070	1 2 0 1 1	
2.551E-01	5.570E+01	25.00	H031	1 2 2 2 2	
2.299E-01	5.020E+01	27.00	H032	1 1 2 1 2	
2.244E-01	4.900E+01	27.8	H032	1 1 2 1 2	
2.125E-01	4.640E+01	29.0	H032	1 1 2 1 2	
2.020E-01	4.410E+01	30.2	H032	1 1 2 1 2	
1.974E-01	4.310E+01	31.1	H032	1 1 2 1 2	
1.892E-01	4.130E+01	32.0	H032	1 1 2 1 2	
1.818E-01	3.970E+01	32.5	H032	1 1 2 1 2	
1.626E-01	3.550E+01	34.50	H031	1 2 2 2 2	
1.530E-01	3.340E+01	36.0	H032	1 1 2 1 2	
1.205E-01	2.630E+01	42.6	H032	1 1 2 1 2	
1.063E-01	2.320E+01	46.0	H032	1 1 2 1 2	
1.035E-01	2.260E+01	46.70	H031	1 2 2 2 2	
8.932E-02	1.950E+01	50.4	H032	1 1 2 1 2	
7.466E-02	1.630E+01	56.00	H031	1 2 2 2 2	
5.176E-02	1.130E+01	76.50	H031	1 2 2 2 2	
4.306E-02	9.400E+00	99.00	H031	1 2 2 2 2	

2980. $C_{12}H_{27}O_2P$
Butyl dibutyl phosphinate
Butoxydibutylphosphine oxide
Dibutylbutoxyphosphine oxide
Butyl dibutylphosphinate
RN: 2950-47-2 **MP** (°C)**:**
MW: 234.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	4.500E+00	25	B070	1 2 0 1 1	

2981. $C_{12}H_{27}O_3P$
Diethyl octyl phosphonate
Diethyl octanephosphonate
RN: 1068-07-1 **MP** (°C)**:**
MW: 250.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.99E-04	<2.00E-01	25	B070	1 2 0 1 0	

2982. $C_{12}H_{27}O_3P$
Dibutyl butyl phosphonate
Dibutoxybutylphosphine oxide
Dibutyl butanephosphonate
Dibutyl butylphosphonate
TC 44
RN: 78-46-6 **MP** (°C)**:**
MW: 250.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.000E-01	25	B070	1 2 0 1 0	

2983. $C_{12}H_{27}O_4P$
Tributyl phosphate
Tri-*n*-butyl phosphate
RN: 126-73-8 **MP** (°C)**:**
MW: 266.32 **BP** (°C)**:** 289.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-03	1.075E+00	3.4	H027	2 1 2 2 2	
3.800E-03	1.012E+00	4.0	H027	2 1 2 2 2	
3.593E-03	9.570E-01	5.0	H027	2 1 2 2 2	
2.403E-03	6.400E-01	13.0	H027	2 1 2 2 2	
1.500E-03	3.995E-01	25	B070	1 2 0 1 2	
1.464E-03	3.900E-01	25	B070	1 2 0 1 1	

(*continued*)

2983. $C_{12}H_{27}O_4P$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.253E-02	6.000E+00	25	F300	1 0 0 0 0	
1.585E-03	4.220E-01	25.0	H027	2 1 2 2 2	
1.570E-03	4.180E-01	25.0	H032	2 2 2 1 1	EFG
1.070E-03	2.850E-01	50.0	H027	2 1 2 2 2	
1.239E-03	3.299E-01	ns	F014	0 0 0 0 1	

2984. $C_{12}H_{28}Ge$

Tetrapropylgermanium
Tetra-*n*-propylgermane
RN: 994-65-0 **MP** (°C)**:**
MW: 244.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.320E-08	8.133E-06	25	D346	1 1 2 2 2	

2985. $C_{12}Br_{10}O$

Decabromodiphenyl ether
DBDPO
Decabromodiphenyl oxide
RN: 1163-19-5 **MP** (°C)**:** 298.0
MW: 959.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.606E-08	2.500E-05	25	N326	1 0 0 0 1	average

2986. $C_{12}Cl_8O_2$

Octachlorodibenzo-*p*-dioxin
OCDD
1,2,3,4,6,7,8,9-Octachlorodibenzodioxin
O8CDD
Octachlorodibenzo[b,e][1,4]dioxin
RN: 3268-87-9 **MP** (°C)**:** 330
MW: 459.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-13	4.000E-10	20	F303	1 2 1 2 0	
8.700E-13	4.000E-10	20	W319	1 2 1 2 1	
1.610E-13	7.400E-11	25	S352	2 2 0 2 1	
1.610E-13	7.402E-11	25.0	D330	2 2 1 2 2	
4.350E-12	2.000E-09	40	F303	1 2 1 2 1	
4.350E-12	2.000E-09	40	W319	1 2 1 2 1	
6.750E-13	3.103E-10	40.0	D330	2 2 1 2 2	
3.960E-12	1.821E-09	60.0	D330	2 2 1 2 2	
1.710E-12	7.862E-10	80.0	D330	2 2 1 2 2	
8.374E-13	3.850E-10	ns	W332	0 1 0 2 2	

2987. $C_{12}Cl_{10}$
Decachlorobiphenyl
Decachlorbiphenyl
2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl
RN: 2051-24-3 **MP** (°C)**:** 305
MW: 498.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.211E-11	2.100E-08	22	O311	2 2 1 2 1	
1.300E-12	6.483E-10	25	D331	2 1 2 2 2	
1.303E-11	6.500E-09	25	D335	1 0 0 0 1	
1.490E-11	7.430E-09	25	M342	1 0 1 1 2	
3.209E-11	1.600E-08	25	W025	1 0 2 2 1	
1.300E-12	6.483E-10	25.0	M324	1 2 1 1 2	
1.680E-11	8.378E-09	60	D331	2 1 2 2 2	
1.680E-11	8.378E-09	60.0	M324	1 2 1 1 2	
3.530E-11	1.760E-08	70	D331	2 1 2 2 2	
3.530E-11	1.760E-08	70.0	M324	1 2 1 1 2	
9.930E-11	4.952E-08	80	D331	2 1 2 2 2	
9.930E-11	4.952E-08	80.0	M324	1 2 1 1 2	

2988. $C_{13}H_6Cl_5NO_3$
Oxyclozanide
3,5,6,3′,5′-Pentachloro-2,2′-dihydroxybenzanilide
Zanilox
Diplin
ICI 46638
Zanil
RN: 2277-92-1 **MP** (°C)**:**
MW: 401.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.224E-05	2.900E-02	25	P036	0 0 0 0 0	average of 3, form III
2.665E-06	1.070E-03	25	P036	0 0 0 0 0	average of 3, form II
6.227E-07	2.500E-04	25	P036	0 0 0 0 0	average of 3, form I

2989. $C_{13}H_6Cl_6O_2$
Hexachlorophene
2,2′-Methylenebis[3,4,6-trichlorophenol]
Bilevon
AT-7
Dermadex
Exofene
RN: 70-30-4 **MP** (°C)**:** 164.5
MW: 406.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.142E-04	2.499E-01	22	M048	1 0 1 1 0	EFG
4.669E-05	1.900E-02	25	A008	1 0 0 0 0	EFG
3.441E-04	1.400E-01	25	A010	2 2 2 1 1	0.003N HCl
7.373E-07	3.000E-04	ns	V302	0 0 0 0 0	*sic*

2990. $C_{13}H_7Br_2N_3O_6$
Bromofenoxim
3,5-Dibromo-4-hydroxybenzaldehyde-2,4-dinitrophenyloxime
Faneron
Bromfenim
RN: 13181-17-4 **MP** (°C)**:** 196.5
MW: 461.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.169E-07	1.000E-04	20	M161	1 0 0 0 0	
1.288E-06	5.939E-04	ns	R427	0 0 0 0 0	

2991. $C_{13}H_7F_3N_2O_5$
Fluorodifen
p-Nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether
RN: 15457-05-3 **MP** (°C)**:** 90
MW: 328.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.094E-06	2.000E-03	20	E048	1 2 1 1 0	
6.094E-06	2.000E-03	20	M161	1 0 0 0 0	
<6.09E-06	<2.00E-03	ns	B200	0 0 0 0 0	
6.094E-06	2.000E-03	ns	M061	0 0 0 0 0	

2992. $C_{13}H_8ClFO_2$
4′-Chloro-5-fluoro-2-hydroxy benzophenone
SL 79182
RN: 62433-26-5 **MP** (°C)**:**
MW: 250.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-05	8.999E-03	37	F309	1 0 2 2 2	

2993. $C_{13}H_8ClNO$
CP 31675
2-Chloro-*N*-(2-methyl-6-*t*-butylphenyl)acetamide
RN: 3785-20-4 **MP** (°C)**:** 115
MW: 229.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.306E-03	3.000E-01	ns	M061	0 0 0 0 2	

2994. $C_{13}H_8ClN_3O$
RJ-64
3,4-Pyridyl-(5)-2-chlorophenyl-1,2,4-oxadiazole
RN: 27199-40-2 **MP** (°C)**:**
MW: 257.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.045E-03	1.300E+00	37	C054	2 2 2 1 2	0.1N HCl

2995. $C_{13}H_8Cl_2N_2O_4$
Niclosamide
2′,5-Dichloro-4′-nitrosalicylanilide
2-Chloro-4-nitrophenylamide-6-chlorosalicylic acid
Cestocid
Devermine
Bayluscid
RN: 50-65-7 **MP** (°C)**:** 230
MW: 327.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-05	1.332E-02	25	T426	0 0 0 0 0	
1.987E-05	6.500E-03	rt	M161	0 0 0 0 0	

2996. $C_{13}H_8F_2O_3$
Diflunisal
5-(2,4-Difluorophenyl) salicylic acid
Dolobid
RN: 22494-42-4 **MP** (°C)**:**
MW: 250.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-05	6.186E-03	24.99	K447	0 0 0 0 0	pH 2.0
1.199E-05	3.000E-03	37	Y421	0 0 0 0 0	

2997. $C_{13}H_8N_2O_2$
Phenazine-1-carboxylic acid
PCA
RN: **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-04	5.157E-02	5.0	Y409	0 0 0 0 0	
2.300E-04	5.157E-02	10.0	Y409	0 0 0 0 0	
2.400E-04	5.381E-02	15.0	Y409	0 0 0 0 0	
2.500E-04	5.606E-02	20.0	Y409	0 0 0 0 0	

(*continued*)

2997. $C_{13}H_8N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	6.054E-02	25.0	Y409	0 0 0 0 0	
2.900E-04	6.502E-02	30.0	Y409	0 0 0 0 0	
3.200E-04	7.175E-02	35.0	Y409	0 0 0 0 0	
3.500E-04	7.848E-02	40.0	Y409	0 0 0 0 0	
3.900E-04	8.745E-02	45.0	Y409	0 0 0 0 0	
4.400E-04	9.866E-02	50.0	Y409	0 0 0 0 0	
5.100E-04	1.144E-01	55.0	Y409	0 0 0 0 0	

2998. $C_{13}H_8N_2O_2S$

m-Pyridine carboxyphenylisothiocyanate
Picolinic acid, *m*-isothiocyanatophenyl ester
RN: 5174-37-8 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.281E-02	25	K032	2 2 0 1 1	

2999. $C_{13}H_9ClN_2O_4$

4′-Chloro-2-hydroxy-3-nitrobenzanilide
Salicylanilide, 4′-chloro-5-nitro-
Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-5nitro-
RN: 6490-98-8 **MP** (°C)**:** 253–254
MW: 292.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-06	2.210E-03	25	D400	2 0 0 1 2	

3000. $C_{13}H_9ClN_2O_4$

4′-Chloro-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-3-nitro-
Salicylanilide, 4′-chloro-3-nitro-
NSC 22899
4′-Chloro-3-nitrosalicylanilide
RN: 6490-99-9 **MP** (°C)**:**
MW: 292.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.851E-05	8.344E-03	25	D400	2 0 0 1 2	

3001. $C_{13}H_9Cl_2NO_4$
2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether
Chlomethoxyfen
Chlomethoxynil
RN: 32861-85-1 **MP** (°C)**:** 113.5
MW: 314.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.550E-07	3.000E-04	15	M161	1 0 0 0 0	

3002. $C_{13}H_9F_3N_2O_2$
Niflumic acid
2-[3-(Trifluoromethyl)anilino]nicotinic acid
Actol
Flogovital
Donalgin
Landruma
RN: 4394-00-7 **MP** (°C)**:** 204
MW: 282.22 **BP** (°C)**:** 378.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-04	7.714E-02	10	B429	1 0 1 2 2	
2.805E-04	7.917E-02	15	B429	1 0 1 2 2	
2.916E-04	8.231E-02	20	B429	1 0 1 2 2	
3.028E-04	8.544E-02	25	B429	1 0 1 2 2	
3.128E-04	8.827E-02	30	B429	1 0 1 2 2	
3.261E-04	9.203E-02	35	B429	1 0 1 2 2	
6.732E-05	1.900E-02	rt	H302	0 0 2 1 1	intrinsic
1.400E-04	3.950E-02	rt	R431	0 0 0 0 0	Average

3003. $C_{13}H_9N$
Phenanthridine
Phenanthridin
9-Azaphenanthrene
3,4-Benzoisoquinoline
5-Azaphenanthrene
RN: 229-87-8 **MP** (°C)**:** 106.5
MW: 179.22 **BP** (°C)**:** 349

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.674E-03	3.000E-01	20	F300	1 0 0 0 1	

3004. $C_{13}H_9N$
Acridine
2,3,5,6-Dibenzopyridine
Acridin
RN: 260-94-6 **MP** (°C)**:** 107
MW: 179.22 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.735E-02	24	A029	2 0 0 0 1	0.01N KOH
2.142E-04	3.840E-02	24	H106	1 0 2 2 2	
2.143E-04	3.840E-02	24	M303	1 0 1 1 2	
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	EFG
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	

3005. $C_{13}H_9NO$
2-Hydroxyacridine
o-Hydroxyacridine
RN: 22817-17-0 **MP** (°C)**:**
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.904E-03	20	A029	1 0 0 0 0	

3006. $C_{13}H_9NS$
p-Biphenyl isothiocyanate
4-Biphenyl isothiocyanate
RN: 25687-48-3 **MP** (°C)**:**
MW: 211.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	2.958E-03	25	D019	1 1 1 1 1	

3007. $C_{13}H_9NS$
m-Biphenyl isothiocyanate
3-Biphenyl isothiocyanate
RN: 1510-25-4 **MP** (°C)**:**
MW: 211.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	6.339E-03	25	K032	2 2 0 1 1	

3008. $C_{13}H_{10}$
Fluorene
o-Biphenylmethane
2,3-Benzindene
o-Biphenylenemethane
Diphenylenemethane
2,2′-Methylenebiphenyl
RN: 86-73-7 **MP** (°C)**:** 116
MW: 166.22 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-06	7.181E-04	6.60	M082	1 1 1 2 2	
4.320E-06	7.181E-04	6.60	M151	2 1 2 2 2	
4.326E-06	7.190E-04	6.64	M183	1 2 1 1 2	
5.820E-06	9.674E-04	13.20	M082	1 1 1 2 2	
5.820E-06	9.674E-04	13.20	M151	2 1 2 2 2	
5.822E-06	9.678E-04	13.24	M183	1 2 1 1 2	
7.240E-06	1.203E-03	18.00	M082	1 1 1 2 2	
7.240E-06	1.203E-03	18.00	M151	2 1 2 2 2	
7.244E-06	1.204E-03	18.04	M183	1 2 1 1 2	
9.012E-06	1.498E-03	20	V416	0 0 0 0 0	
9.720E-06	1.616E-03	24.00	M082	1 1 1 2 2	
9.720E-06	1.616E-03	24.00	M151	2 1 2 2 2	
9.728E-06	1.617E-03	24.04	M183	1 2 1 1 2	
1.137E-05	1.890E-03	24.60	W003	2 2 2 2 2	average of 3
1.179E-05	1.960E-03	25	B319	2 0 1 2 2	
2.790E-05	4.638E-03	25	L301	1 1 2 2 2	
1.143E-05	1.900E-03	25	L332	1 1 1 1 1	
1.191E-05	1.980E-03	25	M064	1 1 2 2 2	
1.014E-05	1.685E-03	25	M071	2 2 2 2 2	
1.190E-05	1.978E-03	25	M342	1 0 1 1 2	
1.010E-05	1.679E-03	25	W300	2 2 2 2 2	
1.014E-05	1.685E-03	25.00	M151	2 1 1 2 2	
1.110E-05	1.845E-03	27.00	M082	1 1 1 2 2	
1.110E-05	1.845E-03	27.00	M151	2 1 2 2 2	
1.111E-05	1.847E-03	27.04	M183	1 2 1 1 2	
1.420E-05	2.360E-03	29.90	W003	2 2 2 2 2	average of 3
1.317E-05	2.190E-03	30.30	W003	2 2 2 2 2	average of 3
1.350E-05	2.244E-03	31.10	M082	1 1 1 2 2	
1.350E-05	2.244E-03	31.10	M151	2 1 2 2 2	
1.353E-05	2.250E-03	31.14	M183	1 2 1 1 2	
2.244E-05	3.730E-03	38.40	W003	2 2 2 2 2	average of 2
2.223E-05	3.695E-03	40	V416	0 0 0 0 0	
2.322E-05	3.860E-03	40.10	W003	2 2 2 2 2	average of 3
3.387E-05	5.630E-03	47.50	W003	2 2 2 2 2	average of 3
3.862E-05	6.420E-03	50.10	W003	2 2 2 2 2	average of 3
3.772E-05	6.270E-03	50.20	W003	2 2 2 2 2	
5.071E-05	8.430E-03	54.70	W003	2 2 2 2 2	average of 3
6.317E-05	1.050E-02	59.20	W003	2 2 2 2 2	
5.298E-05	8.806E-03	60	V416	0 0 0 0 0	
6.678E-05	1.110E-02	60.50	W003	2 2 2 2 2	average of 3

(*continued*)

3008. $C_{13}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.543E-05	1.420E-02	65.10	W003	2 2 2 2 2	average of 3
1.119E-04	1.860E-02	70.70	W003	2 2 2 2 2	average of 3
1.131E-04	1.880E-02	71.90	W003	2 2 2 2 2	
1.293E-04	2.150E-02	73.40	W003	2 2 2 2 2	
1.191E-05	1.980E-03	ns	M344	0 0 0 0 2	

3009. $C_{13}H_{10}BrCl_2O_2PS$

Leptophos
Phenylphosphonothioic acid *O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl ester
Phosvel
NK 711
Velsicol 506
Oleophosvel

RN: 21609-90-5 **MP** (°C)**:** 60
MW: 412.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.280E-09	3.000E-06	10	B324	0 0 0 0 0	
8.707E-09	3.588E-06	10	B324	0 0 0 0 0	
1.699E-07	7.000E-05	20	B169	2 2 1 1 0	
6.095E-08	2.512E-05	20	B300	2 2 1 1 2	
6.095E-08	2.512E-05	20	B324	0 0 0 0 0	
5.096E-08	2.100E-05	20	B324	0 0 0 0 0	
1.141E-08	4.700E-06	20	C053	0 0 0 0 0	
1.213E-08	5.000E-06	22	K137	1 1 2 1 0	
7.280E-08	3.000E-05	24	C105	2 1 2 2 2	
5.824E-06	2.400E-03	25	M161	1 0 0 0 1	*sic*
1.306E-07	5.382E-05	30	B324	0 0 0 0 0	
1.092E-07	4.500E-05	30	B324	0 0 0 0 0	
2.184E-08	9.000E-06	ns	F040	1 2 2 2 0	
1.141E-08	4.700E-06	ns	F071	0 1 2 1 1	
1.699E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG

3010. $C_{13}H_{10}BrCl_2O_3P$

Leptophos oxon
O-(4-Bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphonate
Phosvel oxon

RN: 25006-32-0 **MP** (°C)**:**
MW: 396.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.586E-06	3.400E-03	20.50	B169	2 2 1 1 2	

3011. $C_{13}H_{10}ClNO_2$

4′-Chloro salicylanilide
N-(*p*-Chlorophenyl)-*o*-hydroxybenzamide
N-(*p*-Chlorophenyl)salicylamide
RN: 3679-63-8 **MP** (°C)**:**
MW: 247.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.885E-08	1.210E-05	ns	N336	0 0 0 0 0	intrinsic

3012. $C_{13}H_{10}Cl_2O$

2,4,-Dichloro-6-benzyl-phenol
o-Cresol, 4,6-dichloro-α-phenyl-
2-Benzyl-4,6-dichlorophenol
RN: 19578-81-5 **MP** (°C)**:**
MW: 253.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	5.822E-03	25	B316	0 0 0 0 0	

3013. $C_{13}H_{10}Cl_2O_2$

Dichlorophen
2,2′-Dihydroxy-5,5′-dichlorodiphenylmethane
G-4
RN: 97-23-4 **MP** (°C)**:** 177–178
MW: 269.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-04	3.000E-02	25	M061	1 0 0 0 0	
1.115E-04	3.000E-02	25	M161	1 0 0 0 1	
1.122E-04	3.020E-02	ns	R427	0 0 0 0 0	

3014. $C_{13}H_{10}INO$

Benodanil
2-Iodo-*N*-phenylbenzamide
Iodobenzanilide
Calirus
RN: 15310-01-7 **MP** (°C)**:** 137
MW: 323.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.189E-05	2.000E-02	20	M161	1 0 0 0 1	

3015. $C_{13}H_{10}N_2$
9-Aminoacridine
10-Amino-5-azaanthracene
Monacrin
Izoacridina
Aminacrine
9AA
RN: 90-45-9 **MP** (°C)**:** 241
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 1 0	0.01N KOH

3016. $C_{13}H_{10}N_2$
4-Aminoacridine
4-Acridinamine
RN: 578-07-4 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.360E-02	24	A029	2 0 0 1 0	0.01N KOH

3017. $C_{13}H_{10}N_2$
3-Aminoacridine
3-Acridinamine
RN: 581-29-3 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.914E-02	24	A029	2 0 0 1 1	0.01N KOH

3018. $C_{13}H_{10}N_2$
2-Aminoacridine
2-Acridinamine
RN: 581-28-2 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	9.712E-03	24	A029	2 0 0 1 0	0.01N KOH

3019. $C_{13}H_{10}N_2$
1-Aminoacridine
1-Acridinamine
RN: 578-06-3 **MP** (°C)**:** 183
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 0 1	intrinsic

3020. $C_{13}H_{10}N_4O_3$
1-Benzoyloxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(benzoyloxy)methyl]-1,5-dihydro-
RN: 98846-65-2 **MP** (°C)**:** 217–219
MW: 270.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.881E-05	2.400E-02	22	B322	0 0 0 0 0	
8.913E-05	2.409E-02	ns	R427	0 0 0 0 0	

3021. $C_{13}H_{10}O$
Benzophenone
α-Oxodiphenylmethane
Diphenylmethanone
Benzoylbenzene
α-Oxoditane
Oxoditane
RN: 119-61-9 **MP** (°C)**:** 48.5
MW: 182.22 **BP** (°C)**:** 305.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.121E-04	7.510E-02	20	H301	0 0 0 0 0	
7.500E-04	1.367E-01	25	F063	1 1 0 0 1	
3.292E-04	6.000E-02	ns	F014	0 0 0 0 0	

3022. $C_{13}H_{10}O_3$
2,4-Dihydroxybenzophenone
RN: 131-56-6 **MP** (°C)**:**
MW: 214.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	7.050E+00	19.99	L452	0 0 0 0 0	
4.255E-02	9.116E+00	24.99	L452	0 0 0 0 0	
4.805E-02	1.029E+01	29.99	L452	0 0 0 0 0	
5.672E-02	1.215E+01	34.99	L452	0 0 0 0 0	
7.396E-02	1.584E+01	39.99	L452	0 0 0 0 0	

(*continued*)

3022. $C_{13}H_{10}O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.659E-02	1.855E+01	44.99	L452	0 0 0 0 0	
1.174E-01	2.515E+01	49.99	L452	0 0 0 0 0	
1.500E-01	3.213E+01	54.99	L452	0 0 0 0 0	
1.925E-01	4.123E+01	59.99	L452	0 0 0 0 0	
2.559E-01	5.482E+01	64.99	L452	0 0 0 0 0	
3.498E-01	7.493E+01	69.99	L452	0 0 0 0 0	

3023. $C_{13}H_{10}O_3$

Phenyl salicylate
Salol
2-Hydroxybenzoic acid phenyl ester

RN: 118-55-8 **MP** (°C)**:** 42.0
MW: 214.22 **BP** (°C)**:** 173.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.002E-04	1.500E-01	25	F300	1 0 0 0 1	
7.469E-05	1.600E-02	ns	B404	0 2 1 1 0	
1.866E-03	3.998E-01	rt	D021	0 0 1 1 0	

3024. $C_{13}H_{10}O_4$

2,3,4-Trihydroxybenzophenone
2,3,4-Trihydroxy-benzophenon

RN: 1143-72-2 **MP** (°C)**:**
MW: 230.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.811E-02	1.108E+01	19.99	L452	0 0 0 0 0	
5.743E-02	1.322E+01	24.99	L452	0 0 0 0 0	
8.057E-02	1.855E+01	29.99	L452	0 0 0 0 0	
1.051E-01	2.420E+01	34.99	L452	0 0 0 0 0	
1.392E-01	3.204E+01	39.99	L452	0 0 0 0 0	
1.831E-01	4.215E+01	44.99	L452	0 0 0 0 0	
2.574E-01	5.927E+01	49.99	L452	0 0 0 0 0	
3.440E-01	7.919E+01	54.99	L452	0 0 0 0 0	
4.723E-01	1.087E+02	59.99	L452	0 0 0 0 0	
6.152E-01	1.416E+02	64.99	L452	0 0 0 0 0	
7.804E-01	1.797E+02	69.99	L452	0 0 0 0 0	

3025. $C_{13}H_{10}O_4$

2,4,6-Trihydroxybenzophenone
2,4,6-Trihydroxy-benzophenon
RN: 3555-86-0 **MP** (°C)**:**
MW: 230.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.347E-02	3.100E+00	22	F300	1 0 0 0 1	

3026. $C_{13}H_{10}O_5$

2,2′,4,4′-Tetrahydroxybenzophenone
RN: **MP** (°C)**:**
MW: 246.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.863E-02	7.050E+00	19.99	L452	0 0 0 0 0	
3.583E-02	8.821E+00	24.99	L452	0 0 0 0 0	
4.538E-02	1.117E+01	29.99	L452	0 0 0 0 0	
6.199E-02	1.526E+01	34.99	L452	0 0 0 0 0	
8.431E-02	2.076E+01	39.99	L452	0 0 0 0 0	
1.079E-01	2.657E+01	44.99	L452	0 0 0 0 0	
1.487E-01	3.661E+01	49.99	L452	0 0 0 0 0	
2.190E-01	5.393E+01	54.99	L452	0 0 0 0 0	
3.285E-01	8.088E+01	59.99	L452	0 0 0 0 0	
4.448E-01	1.095E+02	64.99	L452	0 0 0 0 0	
5.572E-01	1.372E+02	69.99	L452	0 0 0 0 0	

3027. $C_{13}H_{10}O_5$

2,3,4,4′-Tetrahydroxybenzophenone
RN: 31127-54-5 **MP** (°C)**:**
MW: 246.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.578E-02	1.127E+01	19.99	L452	0 0 0 0 0	
6.120E-02	1.507E+01	24.99	L452	0 0 0 0 0	
8.820E-02	2.172E+01	29.99	L452	0 0 0 0 0	
1.202E-01	2.960E+01	34.99	L452	0 0 0 0 0	
1.712E-01	4.215E+01	39.99	L452	0 0 0 0 0	
2.299E-01	5.660E+01	44.99	L452	0 0 0 0 0	
3.216E-01	7.919E+01	49.99	L452	0 0 0 0 0	
4.768E-01	1.174E+02	54.99	L452	0 0 0 0 0	
6.166E-01	1.518E+02	59.99	L452	0 0 0 0 0	
8.432E-01	2.076E+02	64.99	L452	0 0 0 0 0	
1.084E+00	2.669E+02	69.99	L452	0 0 0 0 0	

3028. $C_{13}H_{10}O_6$
Maclurin
2,4,6,3′,4′-Penta-hydroxy-benzophenol
2,4,6,3′,4′-Pentahydroxybenzophenon
RN: 519-34-6 **MP** (°C)**:** 222.5
MW: 262.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-02	5.000E+00	14	F300	1 0 0 0 0	

3029. $C_{13}H_{11}ClF_3N_3O$
San 6706
4-Chloro-5-(dimethylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3(2H)-pyridazinone
RN: 23576-23-0 **MP** (°C)**:** 151
MW: 317.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.305E-05	1.050E-02	23.50	B200	2 0 0 0 2	

3030. $C_{13}H_{11}ClN_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-
RN: 134698-40-1 **MP** (°C)**:**
MW: 274.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-06	1.199E-03	ns	M381	0 1 1 1 2	pH 7.0

3031. $C_{13}H_{11}ClO$
Chlorophene
5-Chloro-2-hydroxydiphenylmethane
Benzylchlorophenol
RN: 120-32-1 **MP** (°C)**:** 48.5
MW: 218.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	4.155E+00	20	A008	1 0 0 0 0	EFG
1.100E-01	2.406E+01	ns	B047	0 0 0 0 0	EFG

3032. $C_{13}H_{11}N$
2-Aminofluorene
9H-Fluoren-2-amine
2-Fluorenamine
RN: 153-78-6 **MP** (°C)**:** 129
MW: 181.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	3.100E-02	rt	N015	0 0 2 2 1	

3033. $C_{13}H_{11}NO_2$
Salicylanilide
2-Hydroxy-*N*-phenylbenzamide
2-Hydroxybenzanilide
RN: 87-17-2 **MP** (°C)**:** 136
MW: 213.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.579E-04	5.500E-02	23	M061	1 0 0 0 1	
2.579E-04	5.500E-02	25	M161	1 0 0 0 1	

3034. $C_{13}H_{11}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,7-dimethyl-
RN: 74103-12-1 **MP** (°C)**:**
MW: 229.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.597E-08	2.200E-05	25	P089	0 0 0 0 0	
1.527E-07	3.500E-05	37	P089	0 0 0 0 0	
2.116E-07	4.850E-05	51	P089	0 0 0 0 0	

3035. $C_{13}H_{11}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,6-dimethyl-
RN: **MP** (°C)**:**
MW: 229.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-07	5.800E-05	25	P089	0 0 0 0 0	
3.054E-07	7.000E-05	37	P089	0 0 0 0 0	
3.817E-07	8.750E-05	51	P089	0 0 0 0 0	

3036. $C_{13}H_{11}NO_5$
Oxolinic acid
5-Ethyl-5,8-dihydro-8-oxo-1,3-dioxolo(4,5-g)quinoline-7-carboxylic acid
Dioxacin
Gramurin
Starner
S-0208
RN: 14698-29-4 **MP** (°C)**:**
MW: 261.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.214E-03	ns	R427	0 0 0 0 0	

3037. $C_{13}H_{11}N_3O_2$
Benquinox
Cerenox
Seredon
Benzoylhydrazone of quinone oxime
RN: 495-73-8 **MP** (°C)**:**
MW: 241.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-05	5.000E-03	ns	M061	0 0 0 0 0	

3038. $C_{13}H_{11}N_3O_2S_2$
2-Sulfanilamidobenzothiazole
RN: **MP** (°C)**:**
MW: 305.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.275E-06	1.000E-03	37	R045	1 2 1 1 1	

3039. $C_{13}H_{11}N_3O_4S_2$
Tenoxicam
Mobiflex
RN: 59804-37-4 **MP** (°C)**:**
MW: 337.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-04	6.190E-02	32	C411	2 1 1 2 1	

3040. $C_{13}H_{11}N_7O_4S$

5-*p*-Nitrobenzenesulfonamidotetrazole

RN: **MP** (°C)**:**
MW: 361.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.214E-05	8.000E-03	37	R045	1 2 1 1 0	

3041. $C_{13}H_{11}O_3P$

4-Carboxyethylphenylphenylphosphinic acid
CPPPA

RN: **MP** (°C)**:**
MW: 246.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.399E-02	3.443E+00	-239.0	W412	0 0 0 0 0	
1.242E-02	3.059E+00	26.7	W412	0 0 0 0 0	
1.676E-02	4.127E+00	45.08	W412	0 0 0 0 0	
1.931E-02	4.754E+00	54.4	W412	0 0 0 0 0	
2.609E-02	6.424E+00	64.15	W412	0 0 0 0 0	
3.477E-02	8.561E+00	75.71	W412	0 0 0 0 0	
4.371E-02	1.076E+01	84.38	W412	0 0 0 0 0	
3.780E+00	9.307E+02	94.52	W412	0 0 0 0 0	

3042. $C_{13}H_{12}$

Diphenylmethane
1,1′-Methylenebis-benzene
Phenylbenzyl
Benzylbenzene

RN: 101-81-5 **MP** (°C)**:** 25.9
MW: 168.24 **BP** (°C)**:** 264.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-05	3.000E-03	24	H116	2 1 0 0 2	
8.381E-05	1.410E-02	25	A001	1 2 2 2 2	
8.381E-05	1.410E-02	25	A017	1 0 0 0 2	
8.710E-05	1.465E-02	25	D001	1 0 0 0 2	

3043. $C_{13}H_{12}$
4-Methylbiphenyl
4-Phenyltoluene
RN: 644-08-6 **MP** (°C)**:** 49.5
MW: 168.24 **BP** (°C)**:** 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-05	1.834E-03	4.9	D330	2 2 1 2 2	
2.410E-05	4.055E-03	25.0	D330	2 2 1 2 2	
4.180E-05	7.032E-03	40.0	D330	2 2 1 2 2	

3044. $C_{13}H_{12}F_2N_6O$
Fluconazole
1H-1,2,4-Triazole-1-ethanol, α(2,4-difluorophenyl)-α-(1H-1,2,4-triazol-1-ylmethyl)
2,4-Difluoro-α,α1-bis(1H-1,2,4-triazol-1-ylmethyl)benzyl alcohol
Diflucan
Triflucan
RN: 86386-73-4 **MP** (°C)**:** 138–140
MW: 306.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.265E-03	1.000E+00	ns	K444	0 0 0 0 0	

3045. $C_{13}H_{12}N_2O$
Carbanilide
Diphenylurea
N,N′-Diphenylurea
RN: 102-07-8 **MP** (°C)**:** 238.0
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-04	1.503E-01	ns	R427	0 0 0 0 0	
7.066E-04	1.500E-01	rt	D021	0 0 1 1 1	

3046. $C_{13}H_{12}N_2O_3$
Phenallymal
5-Allyl-5-phenylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-phenyl-5-(2-propenyl)
Barbituric acid, 5-allyl-5-phenyl
5-Allyl-5-phenylbarbiturate
RN: 115-43-5 **MP** (°C)**:** 156.5
MW: 244.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.499E-03	1.099E+00	20	J030	1 2 2 2 2	
4.272E-03	1.043E+00	25	P350	0 0 0 0 0	intrinsic
7.764E-03	1.896E+00	37	J030	1 2 2 2 2	

3047. $C_{13}H_{12}N_2O_5S$
Nimesulide
N-(4-Nitro-2-phenoxyphenyl)-methanesulfonamide
RN: 51803-78-2 **MP** (°C)**:**
MW: 308.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.400E-02	25	S415	0 0 0 0 0	
7.395E-05	2.280E-02	37	P432	0 0 0 0 0	

3048. $C_{13}H_{12}O$
p-Benzylphenol
4-Benzylphenol
RN: 101-53-1 **MP** (°C)**:** 81.5
MW: 184.24 **BP** (°C)**:** 322

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.427E-04	9.999E-02	25	L021	1 0 0 0 0	

3049. $C_{13}H_{12}O$
o-Benzylphenol
2-Benzylphenol
RN: 28994-41-4 **MP** (°C)**:** 53.5
MW: 184.24 **BP** (°C)**:** 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.085E-03	2.000E-01	25	L021	1 0 0 0 0	

3050. $C_{13}H_{12}O$
Benzhydrol
Diphenylmethanol
RN: 91-01-0 **MP** (°C)**:** 69
MW: 184.24 **BP** (°C)**:** 298

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.714E-03	5.000E-01	20	F300	1 0 0 0 0	
2.800E-03	5.159E-01	25	D007	2 0 1 1 1	

3051. $C_{13}H_{12}O_5$
bis(4-Hydroxy-3-coumarin) acetic acid ethyl ester
RN: 548-00-5 **MP** (°C)**:**
MW: 248.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.188E-04	5.431E-02	ns	R427	0 0 0 0 0	

3052. $C_{13}H_{13}Cl_2N_3O_3$
Glycophen
1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-*N*-(1-methylethyl)-2,4-dioxo-
Iprodial
LFA 2043
Iprodione
RN: 36734-19-7 **MP** (°C)**:** 136
MW: 330.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.937E-05	1.300E-02	20	M161	1 0 0 0 1	

3053. $C_{13}H_{13}NO_2$
α-(β-Naphthyl)-α-alanine
Alanine, 3-(1(4H)-naphthylidene)-
RN: 13913-40-1 **MP** (°C)**:**
MW: 215.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-03	4.865E-01	25	M097	2 2 2 2 2	

3054. $C_{13}H_{13}NO_5$
2-Azetidinecarboxylic acid, 1-[(benzoyloxy)acetyl]-
RN: 115178-74-0 **MP** (°C)**:** 149.5
MW: 263.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.217E-03	1.900E+00	22	N317	1 1 2 1 2	

3055. $C_{13}H_{13}N_3O_3S$

*N*4-Acetyl sulfapyridine
Acetylsulfapyridine
Sulfapyridine acetylee
RN: 19077-98-6 **MP** (°C)**:**
MW: 291.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.098E-03	3.200E-01	37	D084	1 0 1 0 1	
7.207E-04	2.100E-01	37	F075	1 0 2 2 2	
1.119E-03	3.260E-01	37	M057	1 0 0 0 2	pH 5.5

3056. $C_{13}H_{13}N_3O_5S_2$

Succinylsulfathiazole
2-(*N*(4)-Succinylsulfanilamido)thiazole
p-2-Thiazolylsulfamoylsuccinanilic acid
Kaoxidin
Colistatin
Cremosuxidine
RN: 116-43-8 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-03	4.900E-01	38	K006	1 0 0 0 1	

3057. $C_{13}H_{13}O_4P$

Diphenyl methyl phosphate
Methyl diphenyl phosphate
RN: 115-89-9 **MP** (°C)**:**
MW: 264.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.633E-06	9.600E-04	24	H116	2 1 0 0 2	*sic*
7.569E-03	2.000E+00	25	A044	1 0 0 0 0	*sic*

3058. $C_{13}H_{14}$

1,4,5-Trimethylnaphthalene
Naphthalene, 1,4,5-trimethyl-
RN: 2131-41-1 **MP** (°C)**:** 58
MW: 170.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-05	2.100E-03	25	M064	1 1 2 2 1	
1.190E-05	2.026E-03	25	M342	1 0 1 1 2	
1.233E-05	2.100E-03	ns	M344	0 0 0 0 1	

3059. $C_{13}H_{14}F_3N_3O_4$
Ethalfluralin
N-Ethyl-*N*-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine
Buvilan
Solanan
RN: 55283-68-6 **MP** (°C)**:** 55.5
MW: 333.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.001E-07	2.000E-04	25	M161	1 0 0 0 0	pH 7
9.002E-07	3.000E-04	ns	D304	1 0 0 0 0	

3060. $C_{13}H_{14}N_2$
4,4′-Methylenedianiline
4,4′-Methylenebisbenzeneamine
Tonox
HT 972
RN: 101-77-9 **MP** (°C)**:** 93
MW: 198.27 **BP** (°C)**:** 398

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.044E-03	1.000E+00	19	I307	0 0 0 0 0	

3061. $C_{13}H_{14}N_2O_3$
Mephobarbital
5-Ethyl-1-methyl-5-phenylbarbituric acid
5-Ethyl-*N*-methyl-5-phenylbarbituric acid
Mebaral
Prominal
Methylphenobarbital
RN: 115-38-8 **MP** (°C)**:** 176
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-04	1.500E-01	20	J030	1 2 2 2 1	
4.872E-04	1.200E-01	37	J030	1 2 2 2 1	

3062. $C_{13}H_{14}N_2O_6$
Benzoic acid, 2-(acetyloxy)-, 2-[(2-amino-2-oxoethyl)amino]-2-oxoethyl ester
RN: 118247-02-2 **MP** (°C)**:** 186
MW: 294.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-03	8.800E-01	21	N335	0 0 0 0 0	

3063. $C_{13}H_{14}N_4$

Pyridine-2-azo-*p*-dimethylaniline
PADA
2-(*p*-*N*,*N*-Dimethylaminophenylazo)pyridine
p-(2-Pyridylazo)-*N*,*N*-dimethylaniline
N,*N*-Dimethyl-4-(2-pyridylazo)aniline
2-(*p*-*N*,*N*-Dimethylaminophenylazo)pyridine
RN: 13103-75-8 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:** 392.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-05	2.127E-02	ns	B418	0 2 1 1 2	

3064. $C_{13}H_{14}N_4O_3S$

*N*4-Acetylsulfamerazine
*N*4-Acetylsulphamerazine
2-*N*4-Acetylsulfanilamido-4-methylpyrimidine
RN: 127-73-1 **MP** (°C)**:**
MW: 306.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.676E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
2.579E-03	7.900E-01	37	L091	1 0 0 0 1	pH 5.5
9.140E-04	2.800E-01	37	R045	1 2 1 1 2	
9.140E-04	2.800E-01	37	R045	1 2 1 1 1	
1.234E-03	3.780E-01	37	S192	1 0 1 1 2	pH 6.0
2.611E-03	8.000E-01	38	K006	1 0 0 0 1	

3065. $C_{13}H_{14}N_4O_4S$

Acetyl sulfamethoxypyridazine
3-(*N*1-Acetylsulfanilamido)-6-methoxypyridazine
Acetylmidicel
RN: 127-75-3 **MP** (°C)**:**
MW: 322.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.825E-04	2.200E-01	37	B046	1 0 2 2 1	pH 4.5

3066. $C_{13}H_{14}O_6$

Salicylic acid acetate, hydroxymethyl ester propionate
RN: 32620-70-5 **MP** (°C)**:** 51.5
MW: 266.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.629E-03	7.000E-01	21	N335	0 0 0 0 0	

3067. $C_{13}H_{14}O_6$
Methylphthalyl ethyl glycolate
2-Ethoxy-2-oxoethyl methyl ester
RN: 85-71-2 **MP** (°C)**:** <–35
MW: 266.25 **BP** (°C)**:** 189

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-03	5.297E-01	20	F070	1 0 0 0 2	

3068. $C_{13}H_{15}NO_2$
Glutethimide
Doriden
Noxyron
RN: 77-21-4 **MP** (°C)**:** 84
MW: 217.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.372E-03	9.500E-01	27	B043	1 0 1 2 0	EFG
4.600E-03	9.994E-01	30	D010	1 2 1 1 2	
4.603E-03	1.000E+00	32	B043	1 0 1 2 0	EFG
5.753E-03	1.250E+00	37	B043	1 0 1 2 0	EFG
5.523E-05	1.200E-02	37	B045	1 0 1 1 2	
4.603E-03	1.000E+00	ns	A090	0 0 0 0 1	*sic*
4.600E-03	9.994E-01	ns	R010	0 1 0 0 2	

3069. $C_{13}H_{15}NO_2$
Pyracarbolid
3,4-Dihydro-6-methyl-*N*-phenyl-2H-pyran-5-carboxamide
Sicarol
RN: 24691-76-7 **MP** (°C)**:** 110.5
MW: 217.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.762E-03	6.000E-01	40	M161	1 0 0 0 0	

3070. $C_{13}H_{15}NO_2S$
m-Carboxylpentylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 249.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-05	1.820E-02	25	K032	2 2 0 1 1	

3071. $C_{13}H_{15}NO_3$
Pyrrolidine, 1-[(benzoyloxy)acetyl]-
RN: 115178-67-1 **MP** (°C)**:** 58
MW: 233.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.701E-02	6.300E+00	22	N317	1 1 2 1 2	

3072. $C_{13}H_{15}NO_4$
Morpholine, 4-[(benzoyloxy)acetyl]-
RN: 106231-68-9 **MP** (°C)**:** 103.5
MW: 249.27 **BP** (°C)**:** 453.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-02	4.200E+00	22	B427	1 0 0 1 1	
1.685E-02	4.200E+00	22	N317	1 1 2 1 2	

3073. $C_{13}H_{15}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(dimethylamino)-2-oxoethyl ester
RN: 118247-04-4 **MP** (°C)**:** 75.5
MW: 265.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-02	7.500E+00	21	N335	0 0 0 0 0	

3074. $C_{13}H_{15}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(ethylamino)-2-oxoethyl ester
RN: 118247-01-1 **MP** (°C)**:** 80.5
MW: 265.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-02	5.520E+00	21	N335	0 0 0 0 0	

3075. $C_{13}H_{15}N_3O_2$
Pyrolan
1-Phenyl-3-methylpyrazolyl-5-dimethylcarbamate
RN: 87-47-8 **MP** (°C)**:** 50
MW: 245.28 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.138E-03	1.996E+00	ns	M061	0 0 0 0 0	

3076. $C_{13}H_{15}N_3O_3S$
2-Sulfanilamido-3-ethoxypyridine
Benzenesulfonamide, 4-amino-*N*-(3-ethoxy-2-pyridinyl)-
RN: 71119-19-2 **MP** (°C)**:**
MW: 293.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.011E-04	2.350E-01	37	R058	1 2 1 1 2	

3077. $C_{13}H_{15}N_3O_3S$
5-Sulfanilamido-2-ethoxypyridine
Benzenesulfonamide, 4-amino-*N*-(6-ethoxy-3-pyridinyl)-
RN: 71720-65-5 **MP** (°C)**:**
MW: 293.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-04	3.600E-02	37	R058	1 2 1 1 1	

3078. $C_{13}H_{15}N_3O_4S$
Acetyl sulfisoxazole
*N*1-Acetyl-sulfaisoxazole
RN: 80-74-0 **MP** (°C)**:** 193.5
MW: 309.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.586E-04	8.000E-02	37	B046	1 0 2 2 0	pH 4.5
1.199E-04	3.710E-02	37	M117	2 1 1 1 2	pH 6.0

3079. $C_{13}H_{15}N_3O_4S$
*N*1-(3,4-Dimethyl-5-isoxazolyl)-*N*4-acetylsulfanilamide
Acetylsulfadimethylisoxazole
*N*4-Acetylsulfisoxazole
4-*N*-Acetylsulfisoxazole
N-Acetylsulfisoxazole
RN: 4206-74-0 **MP** (°C)**:**
MW: 309.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.450E-02	7.579E+00	37	B110	1 0 2 2 2	pH 6.7

3080. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid 1-ethylpropyl ester
RN: 65267-94-9 **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-05	4.855E-03	ns	M120	0 0 1 1 2	

3081. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-pentyl ester
2,4-D Pentyl ester
Pentyl 2,4-dichlorophenoxyacetate
Amyl 2,4-dichlorophenoxyacetate
RN: 1917-92-6 **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.897E-05	8.436E-03	ns	M120	0 0 1 1 2	

3082. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid 2-methylbutyl ester
RN: **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-05	3.760E-03	ns	M120	0 0 1 1 2	

3083. $C_{13}H_{16}F_3N_3O_4$
Benefin
Benfluralin
RN: 1861-40-1 **MP** (°C)**:** 65
MW: 335.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.98E-06	<1.00E-03	25	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	P028	0 0 0 0 0	
2.088E-04	7.000E-02	ns	M061	0 0 0 0 1	

3084. $C_{13}H_{16}F_3N_3O_4$

Trifluralin
α,α,α-Trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine
RN: 1582-09-8 **MP** (°C)**:** 48.5
MW: 335.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E-05	4.000E-03	20	F311	1 2 2 2 1	
2.419E-05	8.110E-03	22	K137	1 1 2 1 0	
1.730E-06	5.800E-04	25	G319	0 0 0 0 0	
<2.98E-06	<1.00E-03	27	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	P028	0 0 0 0 0	
7.158E-05	2.400E-02	ns	B185	0 0 0 0 0	
1.193E-04	4.000E-02	ns	M061	0 0 0 0 1	
2.088E-06	7.000E-04	ns	M110	0 0 0 0 0	EFG
5.488E-07	1.840E-04	ns	V414	0 0 0 0 0	

3085. $C_{13}H_{16}NO_4PS$

Isoxathion
O,O-Diethyl *O*-5-phenylisoxazol-3-yl phosphorothioate
E-48
Karphos
SI-6711
RN: 18854-01-8 **MP** (°C)**:**
MW: 313.31 **BP** (°C)**:** 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.064E-06	1.900E-03	25	N305	1 0 0 0 1	

3086. $C_{13}H_{16}N_2$

3-(1-Methyl-2-pyrrolidinyl)-indole
RN: **MP** (°C)**:**
MW: 200.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-03	7.030E-01	37	H004	0 0 0 0 0	
3.510E-03	7.030E-01	37	H011	0 0 0 0 0	

3087. $C_{13}H_{16}N_2O_2$

Melatonin
Prime-X
RN: 8041-44-9 **MP** (°C)**:**
MW: 232.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-03	4.344E-01	25	B426	1 1 2 2 2	

3088. $C_{13}H_{16}N_2O_4$
N-Acetyl-L-tyrosinamide acetate
RN: **MP** (°C)**:**
MW: 264.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	3.436E+00	25	A066	1 0 1 1 1	

3089. $C_{13}H_{16}N_2O_4$
Methyl-2-ethyl-2-phenylmalonurate
Methyl 2-ethyl-2-phenylmalonurate
RN: 73632-81-2 **MP** (°C)**:** 105
MW: 264.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.757E-01	23	B152	1 2 1 1 1	pH 3.5

3090. $C_{13}H_{16}N_2O_6$
Medinoterb acetate
m-Cresol, 6-*tert*-butyl-2,4-dinitro-, acetate
MC 1488
RN: 2487-01-6 **MP** (°C)**:** 86.5
MW: 296.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.375E-05	1.000E-02	rt	M161	0 0 0 0 1	

3091. $C_{13}H_{16}N_4O_2S$
2-Sulfanilylamino-4-ethyl-5-methylpyrimidine
RN: **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.551E-04	2.500E-01	37	R076	1 2 0 0 1	

3092. $C_{13}H_{16}N_4O_2S$
2-*p*-Aminobenzenesulphonamido-4,5,6-trimethylpyrimidine
Sulfanilamide, *N*1-(4,5,6-trimethyl-2-pyrimidinyl)-
RN: 5433-64-7 **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.131E-04	1.500E-01	37	R075	1 0 0 0 1	

3093. $C_{13}H_{16}N_4O_6.0.5H_2O$

9-[5-*O*-(Acetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
2′-Acetyl-6-methoxypurine arabinoside (hemihydrate)
RN: 121032-43-7 **MP** (°C)**:** 174-176
MW: 333.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-02	1.083E+01	37	C348	0 0 0 0 0	pH 7.00
5.310E-02	1.770E+01	37	M378	1 2 1 1 2	pH 7.2

3094. $C_{13}H_{16}O_4$

Diethylacetyl salicylate
Salicylic acid, 2-ethylbutyrate
RN: 100613-21-6 **MP** (°C)**:**
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.616E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 4.00, intrinsic

3095. $C_{13}H_{16}O_6$

Methyl phthalyl ethyl glycollate
RN: **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.096E-03	1.099E+00	15	H069	1 0 1 1 1	
1.975E-03	5.297E-01	ns	F014	0 0 0 0 1	

3096. $C_{13}H_{16}O_7.0.75H_2O$

Helicin (0.75 hydrate)
Salicylaldehyde β-D-glucoside
Benzaldehyde, 2-(β-D-glucopyranosyloxy)-, hydrate (4:3)
RN: 618-65-5 **MP** (°C)**:**
MW: 297.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.505E-02	1.639E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3097. $C_{13}H_{17}ClO_3$
MCPB-ethyl
RN: 10443-70-6 **MP** (°C)**:**
MW: 256.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.899E-05	1.001E-02	ns	S460	0 0 0 0 0	

3098. $C_{13}H_{17}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-butanoate
5′-Butyryl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-butyrate
RN: 84043-26-5 **MP** (°C)**:** 145.5
MW: 424.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E+03	6.151E+05	25	N332	0 0 0 0 0	pH 7.4

3099. $C_{13}H_{17}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-(2-methylpropanoate)
5′-Isobutyryl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-isobutyrate
RN: 84043-27-6 **MP** (°C)**:** 144.5
MW: 424.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E+03	7.423E+05	25	N332	0 0 0 0 0	pH 7.4

3100. $C_{13}H_{17}NO$
N-Butylcinnamamide
N-Butyl-3-phenyl-2-propenamide
RN: 6299-56-5 **MP** (°C)**:**
MW: 203.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	1.972E-01	ns	H350	0 0 0 0 0	

3101. $C_{13}H_{17}NO$
N,N-Diethylcinnamamide
N,N-Diethyl-3-phenyl-2-propenamide
RN: 3680-04-4 **MP** (°C)**:**
MW: 203.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.450E-03	1.514E+00	ns	H350	0 0 0 0 0	

3102. $C_{13}H_{17}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-butyl-
RN: 115193-28-7 **MP** (°C)**:** 69.5
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-03	4.100E-01	22	N317	1 1 2 1 2	

3103. $C_{13}H_{17}NO_3$
N-Acetyl-L-phenylalanine ethyl ester
RN: 2361-96-8 **MP** (°C)**:**
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.550E+00	5	L081	2 1 2 2 2	
1.755E-02	4.130E+00	28	L081	2 1 2 2 2	
2.814E-02	6.620E+00	40	L081	2 1 2 2 2	
3.417E-02	8.040E+00	55	L081	2 1 2 2 2	
7.268E-02	1.710E+01	65	L081	2 1 2 2 2	

3104. $C_{13}H_{17}NO_3$
2-(*p*-Acetaminophenoxy)tetrahydropyran
RN: 51453-65-7 **MP** (°C)**:** 60
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	7.059E-01	ns	H076	0 0 0 0 0	

3105. $C_{13}H_{17}NO_3$
Pivalyl acetaminophen
Propanoic acid, 2,2-dimethyl-, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, pivalate (ester)
RN: 20675-23-4 **MP** (°C)**:** 162.5–163
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.675E-04	1.100E-01	37	D029	0 0 0 0 0	

3106. $C_{13}H_{17}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-(1,1-dimethylethyl)-
RN: 106231-52-1 **MP** (°C)**:** 112–113
MW: 235.29 **BP** (°C)**:** 418.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	B427	1 0 0 1 1	

3107. $C_{13}H_{17}NO_3$

Acetamide, 2-(benzoyloxy)-*N,N*-diethyl-

RN: 64649-63-4 **MP** (°C)**:** 72.5
MW: 235.29 **BP** (°C)**:** 377.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	2.000E+00	22	B427	1 0 0 1 1	in 0.01M HCl
8.500E-03	2.000E+00	22	N317	1 1 2 1 2	

3108. $C_{13}H_{17}NO_3$

Butanamide, 4-(benzoyloxy)-*N,N*-dimethyl-

RN: 115178-78-4 **MP** (°C)**:** 40.5
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.908E-02	1.390E+01	22	N317	1 1 2 1 2	

3109. $C_{13}H_{17}NO_4$

Benzoic acid, 2-hydroxy-, 2-(diethylamino)-2-oxoethyl ester
N,N-Diethylglycolamide salicylate
N,N-Diethyl glycolamide salicylate

RN: 65783-69-9 **MP** (°C)**:** 74–75
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	7.000E-01	21	B331	1 2 2 1 1	pH 7.4
2.786E-03	7.000E-01	21	B331	0 0 0 0 0	

3110. $C_{13}H_{17}NO_4$

Butyl acetaminophen
Carbonic acid, butyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, butyl carbonate (ester)

RN: 19872-68-5 **MP** (°C)**:** 119.5–120
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.367E-04	1.600E-01	37	D029	0 0 0 0 0	

3111. $C_{13}H_{17}NO_4$

Isobutyl acetaminophen
Carbonic acid, isobutyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, isobutyl carbonate (ester)
RN: 20460-96-2 **MP** (°C)**:** 119–121
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.512E-03	3.800E-01	37	D029	0 0 0 0 0	

3112. $C_{13}H_{17}NO_4$

O-(Pivaloyloxymethyl) salicylamide
RN: **MP** (°C)**:** 95
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	1 2 2 1 1	pH 4

3113. $C_{13}H_{17}NO_4$

Propanoic acid, 2,2-dimethyl-, [2-(aminocarbonyl)phenoxy]methyl ester
O-Pivaloyloxymethyl salicylamide
RN: 103951-40-2 **MP** (°C)**:** 94–96
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	0 0 0 0 0	

3114. $C_{13}H_{17}NO_4$

Acetamide, 2-(benzoyloxy)-*N*-ethyl-*N*-(2-hydroxyethyl)-
RN: 106231-60-1 **MP** (°C)**:** 79.5
MW: 251.28 **BP** (°C)**:** 437.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.298E-02	1.080E+01	22	B427	1 0 0 1 1	in 0.01M HCl
4.298E-02	1.080E+01	22	N317	1 1 2 1 2	

3115. $C_{13}H_{17}NO_4$

N-Acetyl-L-tyrosine ethyl ester
Ethyl *N*-acetyl-L-tyrosinate
RN: 840-97-1 **MP** (°C)**:**
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.571E-03	1.400E+00	5	L081	2 1 2 2 2	
1.385E-02	3.480E+00	28	L081	2 1 2 2 2	

3116. $C_{13}H_{17}NO_5$

Acetamide, 2-(benzoyloxy)-*N,N*-bis(2-hydroxyethyl)-

RN: 106231-61-2 **MP** (°C)**:** 81
MW: 267.28 **BP** (°C)**:** 497.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.694E+00	7.200E+02	22	B427	1 0 0 1 1	in 0.01M HCl
2.694E+00	7.200E+02	22	N317	1 1 2 1 2	

3117. $C_{13}H_{17}NO_6$

Acetamide, 2-(benzoyloxy)-*N*-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-

RN: 115193-31-2 **MP** (°C)**:** 126.5
MW: 283.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.401E-02	1.530E+01	22	N317	1 1 2 1 2	

3118. $C_{13}H_{17}N_3O$

Aminopyrine
Amidopyrine
4-Dimethylaminoantipyrine
Febrinina
Febron
Itamidone

RN: 58-15-1 **MP** (°C)**:** 108
MW: 231.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-01	6.540E+01	0	C025	0 0 0 0 2	form A
5.607E-01	1.297E+02	4.62	M109	2 1 1 1 0	EFG
5.463E-01	1.264E+02	10.93	M109	2 1 1 1 0	EFG
5.430E-01	1.256E+02	15.02	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	20	C025	0 0 0 0 2	form A
5.452E-01	1.261E+02	20.96	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	25	P012	0 0 0 0 0	
2.162E-01	5.000E+01	25	P016	1 0 0 1 1	
2.075E-01	4.800E+01	25	P020	2 0 1 1 1	
1.773E+00	4.100E+02	25	P020	2 0 1 1 2	
5.618E-01	1.300E+02	25.35	M109	2 1 1 1 0	EFG
5.965E-01	1.380E+02	29.87	M109	2 1 1 1 0	EFG
2.350E-01	5.436E+01	30	A078	2 1 2 1 0	EFG
2.291E-01	5.300E+01	37	C025	0 0 0 0 2	form A
6.329E-01	1.464E+02	38.37	M109	2 1 1 1 0	EFG
6.646E-01	1.537E+02	49.42	M109	2 1 1 1 0	EFG
3.415E-01	7.900E+01	55	C025	0 0 0 0 2	form A
5.638E-01	1.304E+02	65	C025	0 0 0 0 2	form A
2.162E+00	5.000E+02	69.50	C025	0 0 0 0 2	form A

(*continued*)

3118. $C_{13}H_{17}N_3O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E+00	4.000E+02	70	C025	0 0 0 0 2	form B
1.167E+00	2.700E+02	70.50	C025	0 0 0 0 2	form B
2.879E+00	6.660E+02	74.40	C025	0 0 0 0 2	form B
8.647E-01	2.000E+02	77.50	C025	0 0 0 0 2	form B
6.485E-01	1.500E+02	81	C025	0 0 0 0 2	form B
3.243E+00	7.500E+02	84	C025	0 0 0 0 2	form B
3.359E+00	7.770E+02	92	C025	0 0 0 0 2	form B

3119. $C_{13}H_{17}N_5O_5$

9-(2-*O*-Propionyl-β-D-arabinofuranosyl)adenine

RN: 65174-99-4 **MP** (°C)**:**
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-04	1.170E-01	37	B306	1 2 0 1 2	pH 7.3

3120. $C_{13}H_{17}N_5O_5$

9-[5′-(*O*-Propionyl)-β-D-arabinofuranosyl]adenine ester

RN: 14000-32-9 **MP** (°C)**:** 202.0
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-02	9.200E+00	ns	B134	0 1 1 1 1	

3121. $C_{13}H_{17}N_5O_6$

9-(1,3-Diacetate-2-propoxymethyl)guanine

RN: 86357-19-9 **MP** (°C)**:** 238
MW: 339.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-03	5.800E-01	25	B360	0 0 0 0 0	

3122. $C_{13}H_{17}N_5O_8$

9-(1,3-Dimethoxycarbonyl-2-propoxymethyl)guanine

RN: 91625-66-0 **MP** (°C)**:** 178
MW: 371.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E-04	1.430E-01	25	B360	0 0 0 0 0	

3123. $C_{13}H_{18}ClNO$

Monalide
N-(4-Chlorophenyl)-2,2-dimethylvaleramide
RN: 7287-36-7 **MP** (°C)**:** 87.5
MW: 239.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.510E-05	2.280E-02	23	M161	1 0 0 0 2	
9.510E-05	2.280E-02	ns	M061	0 0 0 0 2	

3124. $C_{13}H_{18}ClNO$

Pentanochlor
Solan
Pentamide, *N*-(3-chloro-4-methylphenyl)-2-methyl-
RN: 2307-68-8 **MP** (°C)**:** 84
MW: 239.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.337E-05	8.000E-03	ns	B185	0 0 0 0 0	
3.545E-05	8.500E-03	rt	M161	0 0 0 0 0	

3125. $C_{13}H_{18}ClN_3O_4S_2$

Cyclopenthiazide
6-Chloro-3-cyclopentylmethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulphonamide 1,1-dioxide
RN: 742-20-1 **MP** (°C)**:** 235
MW: 379.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-04	5.000E-02	rt	A095	0 0 2 2 0	

3126. $C_{13}H_{18}Cl_2N_2O_2$

Melphalan
4-[bis(2-Chloroethyl)amino]-L-phenylalanine
RN: 148-82-3 **MP** (°C)**:**
MW: 305.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	4.400E+00	30	L343	2 1 1 1 0	EFG
5.561E-03	1.697E+00	ns	S469	0 0 0 0 0	

3127. $C_{13}H_{18}N_2O_2$

Lenacil
3-Cyclohexyl-5,6-trimethyleneuracil
RN: 2164-08-1 **MP** (°C)**:** 290
MW: 234.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-05	6.000E-03	25	M061	1 0 0 0 0	
2.561E-05	6.000E-03	25	M161	1 0 0 0 0	

3128. $C_{13}H_{18}N_2O_3$

Heptabarbital
5-(1-Cyclohepten-1-yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-(1-Cyclohepten-1-yl)-5-ethylbarbituric acid
Heptabarbitone
RN: 509-86-4 **MP** (°C)**:** 174
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.503E-01	25	V033	2 0 1 1 2	
1.000E-03	2.503E-01	25.00	T303	1 0 0 0 1	
1.400E-03	3.504E-01	35.00	T303	1 0 0 0 1	
1.170E-02	2.929E+00	40	N008	1 0 1 1 2	*sic*
1.800E-03	4.505E-01	45.00	T303	1 0 0 0 1	

3129. $C_{13}H_{18}N_2O_3S$

Tosylcyclopentylurea
Tosylcyclopentyluree
RN: 1027-87-8 **MP** (°C)**:**
MW: 282.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.649E-04	7.478E-02	37	A028	1 0 2 1 2	intrinsic
2.650E-04	7.483E-02	37	A046	2 0 1 1 2	

3130. $C_{13}H_{18}N_2O_4$

Methyl-2-methyl-2-cyclohexenyl-6-methylmalonurate
Methyl 2-methyl-2-cyclohexenyl-6-methylmalonurate
RN: **MP** (°C)**:** 94
MW: 266.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.592E-01	23	B152	1 2 1 1 1	pH 3.5

3131. $C_{13}H_{18}N_4O_2S_2$

4-Amino-*N*-(5-pentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Benzenesulfonamide, 4-amino-*N*-(5-pentyl-1,3,4-thiadiazol-2-yl)-
RN: 71119-30-7 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	3.656E-02	37	A046	2 0 1 1 2	

3132. $C_{13}H_{18}N_4O_2S_2$

4-Amino-*N*-(5-isopentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Benzenesulfonamide, 4-amino-*N*-[5-(3-methylbutyl)-1,3,4-thiadiazol-2-yl]-
RN: 71119-29-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.938E-02	37	A046	2 0 1 1 2	

3133. $C_{13}H_{18}O_2$

Ibuprofen
2-(4-Isobutylphenyl)propionic acid
Advil
Ebufac
Rufen
RS-Ibuprofen
RN: 15687-27-1 **MP** (°C)**:** 75
MW: 206.29 **BP** (°C)**:** 319.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
3.340E-05	6.890E-03	5	F306	1 0 1 2 2	intrinsic
1.080E-04	2.228E-02	12	B411	1 1 1 2 2	
1.460E-04	3.012E-02	20	B411	1 1 1 2 2	
7.271E-05	1.500E-02	20	N316	1 0 1 1 0	EFG
3.102E-04	6.400E-02	21	B331	1 2 2 1 2	pH 7.4
2.375E-04	4.900E-02	25	A408	2 0 1 2 0	int
1.018E-04	2.100E-02	25	A427	0 0 0 0 0	
5.478E-05	1.130E-02	25	C314	0 0 0 0 0	
5.560E-05	1.147E-02	25	C314	0 0 0 0 0	
9.430E-04	1.945E-01	25	D345	0 0 0 0 0	
4.300E-05	8.870E-03	25	F301	1 1 0 0 1	pH 2.0, *sic*
4.300E-05	8.870E-03	25	F306	1 0 1 2 2	intrinsic
5.520E-05	1.139E-02	25	G431	0 0 0 0 0	
2.424E-04	5.000E-02	25	S450	0 0 0 0 0	Intrinsic
2.090E-04	4.311E-02	29	B411	1 1 1 2 2	
7.505E-05	1.548E-02	30	G431	0 0 0 0 0	
1.212E-04	2.500E-02	30	N316	1 0 1 1 0	EFG

(*continued*)

3133. $C_{13}H_{18}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.970E-05	2.057E-02	35	G431	0 0 0 0 0	
5.210E-05	1.075E-02	37	F306	1 0 1 2 2	intrinsic
1.551E-04	3.200E-02	37	N316	1 0 1 1 0	EFG
5.332E-05	1.100E-02	37	P432	0 0 0 0 0	
2.909E-04	6.000E-02	37	Y421	0 0 0 0 0	
3.040E-04	6.271E-02	38	B411	1 1 1 2 2	
1.281E-04	2.643E-02	40	G431	0 0 0 0 0	
4.760E-04	9.819E-02	47	B411	1 1 1 2 2	
1.600E-04	3.301E-02	50	M335	1 0 2 1 2	pH 5
2.036E-04	4.200E-02	50	N316	1 0 1 1 0	EFG
2.327E-04	4.800E-02	60	N316	1 0 1 1 0	EFG
2.600E-04	5.363E-02	ns	F327	0 0 1 2 2	
4.848E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.018E-04	2.100E-02	rt	H302	0 0 2 1 2	intrinsic
4.096E-04	8.450E-02	rt	R431	0 0 0 0 0	Average

3134. $C_{13}H_{18}O_2$

S-Ibuprofen
(*S*)-(+)-2-(4-Isobutylphenyl)propionic acid
D-Ibuprofen
Seractil
Dexibuprofen

RN: 51146-56-6 **MP** (°C)**:**
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
2.560E-04	5.281E-02	12	B411	1 1 1 2 2	
3.390E-04	6.993E-02	20	B411	1 1 1 2 2	
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	
4.670E-04	9.634E-02	29	B411	1 1 1 2 2	
6.090E-04	1.256E-01	38	B411	1 1 1 2 2	

3135. $C_{13}H_{18}O_2$

r-Ibuprofen
(*R*)-2-(4-Isobutylphenyl)propanoic acid
r-(–)-*p*-Isobutylhydratropic acid
l-Ibuprofen

RN: 51146-57-7 **MP** (°C)**:**
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	

3136. $C_{13}H_{18}O_3$

Hexyl *p*-hydroxybenzoate
4-Hydroxybenzoic acid *N*-hexyl ester
RN: 1083-27-8 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.680E-04	8.180E-02	15	B355	0 0 0 0 0	
3.810E-04	8.469E-02	20	B355	0 0 0 0 0	
6.190E-04	1.376E-01	25	B355	0 0 0 0 0	
1.704E-03	3.789E-01	25	D081	1 2 2 1 2	
3.162E-04	7.029E-02	25	F322	2 0 1 1 0	EFG

3137. $C_{13}H_{18}O_3$

n-Hexyl salicylate
n-Hexyl 2-hydroxybenzoate
RN: 6259-76-3 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-03	2.800E-01	37	D009	1 2 1 1 1	0.1N HCl

3138. $C_{13}H_{18}O_5S$

Ethofumesate
2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate
Nortran
Tramat
RN: 26225-79-6 **MP** (°C)**:** 71
MW: 286.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	5.034E-02	25	H434	0 0 0 0 0	
3.841E-04	1.100E-01	25	M161	1 0 0 0 2	
3.841E-04	1.100E-01	25	W313	1 0 0 0 1	

3139. $C_{13}H_{18}O_7$

Salicin
2-(Hydroxymethyl)phenyl-β-D-glucopyranoside
Salicoside
RN: 138-52-3 **MP** (°C)**:** 199
MW: 286.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	4.000E+01	25	F300	1 0 0 0 0	
9.082E-01	2.600E+02	100	F300	1 0 0 0 1	
1.455E-01	4.167E+01	c	D004	0 0 0 0 0	
8.733E-01	2.500E+02	h	D004	0 0 0 0 0	

3140. $C_{13}H_{19}NO_2$
Hexyl *p*-aminobenzoate
4-Aminobenzoic acid hexyl ester
RN: 55791-76-9 **MP** (°C)**:**
MW: 221.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.302E-02	37	F006	1 1 2 2 2	
4.500E-05	9.959E-03	ns	M066	0 0 0 0 1	
4.300E-05	9.516E-03	rt	B016	0 0 1 1 1	pH 7.4

3141. $C_{13}H_{19}NO_2$
Ibuproxam
2-(4-Isobutylphenyl)propionohydroxamic acid
Ibudros
RN: 53648-05-8 **MP** (°C)**:** 123
MW: 221.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.037E-04	2.000E-01	ns	M148	0 2 0 0 0	

3142. $C_{13}H_{19}NO_4$
N,N-Diethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone
RN: **MP** (°C)**:**
MW: 253.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-01	2.920E+01	20	K050	1 1 1 1 2	

3143. $C_{13}H_{19}NO_4S$
Probenecid
Parabenem
4-((Dipropylamino)sulfonyl)benzoic acid
p-(Dipropylsulfamoyl)benzoic
RN: 57-66-9 **MP** (°C)**:** 195
MW: 285.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E-05	3.600E-03	22.5	B422	2 0 2 2 2	
2.089E-06	5.962E-04	ns	R427	0 0 0 0 0	

3144. $C_{13}H_{19}N_3O_4$

N-(1-Ethylpropyl)-2,6-dinitro-3,4-xylidine
Pendimethalin
RN: 40487-42-1 **MP** (°C)**:** 56.5
MW: 281.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-06	3.000E-04	20	M161	1 0 0 0 0	
1.081E-03	3.040E-01	ns	B185	0 0 0 0 0	
1.066E-06	3.000E-04	ns	V414	0 0 0 0 0	

3145. $C_{13}H_{19}N_3O_6S$

Nitralin
4-(Methylsulfonyl)-2,6-dinitro-*N,N*-dipropylaniline
RN: 4726-14-1 **MP** (°C)**:** 151
MW: 345.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-06	6.000E-04	22	M161	1 0 0 0 0	
1.737E-06	6.000E-04	25	B200	1 0 0 0 0	
1.737E-07	6.000E-05	25	P028	0 0 0 0 0	
1.737E-06	6.000E-04	ns	M061	0 0 0 0 0	

3146. $C_{13}H_{20}N_2O$

Prilocaine
RN: 721-50-6 **MP** (°C)**:**
MW: 220.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	6.169E+00	25	D402	1 2 2 2 0	EFG
2.900E-02	6.389E+00	37	D402	1 2 2 2 0	EFG

3147. $C_{13}H_{20}N_2O_2$

Procaine
Novacaine
Novokain
RN: 59-46-1 **MP** (°C)**:** 60
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	9.453E+00	30	L068	1 0 0 1 0	EFG
4.200E-02	9.925E+00	37.5	L034	2 2 0 1 2	pH 7.4
5.494E-03	1.298E+00	ns	E031	0 0 2 1 2	
2.700E-02	6.381E+00	ns	M066	0 0 0 0 1	

3148. $C_{13}H_{20}N_2O_2$
N,N′-Diethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide
RN: **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.216E-02	7.600E+00	20	K050	1 1 1 1 2	

3149. $C_{13}H_{20}N_2O_2$
4-Aminobenzoic acid-2-(butyl-amino)ethyl ester
2-(Butylamino)ethyl 4-aminobenzoate
RN: **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	4.017E-02	ns	M066	0 0 0 0 1	

3150. $C_{13}H_{20}N_2O_3$
5-Allyl-5-ethylbutylbarbituric acid
RN: **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.587E-02	4.004E+00	20	J030	1 2 2 2 2	
2.579E-02	6.507E+00	37	J030	1 2 2 2 2	

3151. $C_{13}H_{20}N_2O_3$
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1,1-dimethylethyl)-5-(3-methyl-2-butenyl)
5-*t*-Butyl-5-(3-methylbut-2-enyl)barbiturate
RN: 143585-02-8 **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-04	7.090E-02	25	P350	0 0 0 0 0	intrinsic

3152. $C_{13}H_{20}O$
2-Hexyl-6-methylphenol
o-Cresol, 6-hexyl-
RN: 106593-25-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3153. $C_{13}H_{20}O$

2-Hexyl-4-methylphenol
2-Hexyl-*p*-cresol
RN: 54612-53-2 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	6.667E-03	25	L020	1 0 0 0 0	

3154. $C_{13}H_{20}O$

b-Damascone
b-Damascone, *trans*-
trans-2,6,6-Trimethyl-1-crotonylcyclohex-1-ene
trans-*b*-Damascone
Damascone β
RN: 23726-91-2 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	25	D407	1 0 2 2 2	

3155. $C_{13}H_{20}O$

β-Damascone
4-(2,6,6-Trimethyl cyclohex-1-enyl)but-2-en-4-one
Damasione
RN: 23726-92-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	ns	S460	0 0 0 0 0	

3156. $C_{13}H_{20}O$

o-*n*-Heptylphenol
2-*n*-Heptylphenol
RN: 5284-22-0 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.118E-05	1.176E-02	25	L022	1 0 0 0 0	

3157. $C_{13}H_{20}O$
4-Hexyl-2-methylphenol
o-Cresol, 4-hexyl-
RN: 3280-61-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3158. $C_{13}H_{20}O$
α-Ionone
α-Irisone
Cyclocitrylideneacetone
Ionone α
Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
RN: 127-41-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-04	1.059E-01	ns	S460	0 0 0 0 0	

3159. $C_{13}H_{20}O$
p-*n*-Heptylphenol
4-*n*-Heptylphenol
RN: 1987-50-4 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.778E-05	1.111E-02	25	L022	1 0 0 0 0	

3160. $C_{13}H_{21}NO_3$
Salbutamol
Albuterol
Ventolin
RN: 18559-94-9 **MP** (°C)**:** 151
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.771E+01	20	M380	1 0 2 1 0	EFG
7.500E-02	1.795E+01	25	M380	1 0 2 1 0	EFG
7.400E-02	1.771E+01	37	M380	1 0 2 1 0	EFG
5.885E-02	1.408E+01	ns	A092	0 0 0 0 0	

3161. $C_{13}H_{21}O_3PS$

S-Benzyl *O,O*-di-isopropyl phosphorothioate
Isokitazine
Kitazin P
IBP
Iprobenfos
Kitazin L

RN: 26087-47-8 **MP** (°C)**:**
MW: 288.35 **BP** (°C)**:** 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-03	1.000E+00	18	M161	1 0 0 0 0	

3162. $C_{13}H_{21}O_4PS$

4-(Methylthio)phenyl dipropyl phosphate
O,O-Dipropyl *O*-4-methylthiophenyl phosphate
Propaphos
Kayaphos
Kayphosnac

RN: 7292-16-2 **MP** (°C)**:**
MW: 304.35 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.107E-04	1.250E-01	25	M161	1 0 0 0 2	

3163. $C_{13}H_{22}NO_3PS$

Fenamiphos
1-(Methylethyl)-*O*-ethyl-*O*-(3-methyl-4-(methylthio)phenyl)phosphoramidate
Nemacur
Bay 68138

RN: 22224-92-6 **MP** (°C)**:**
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-03	3.059E-01	10	B324	0 0 0 0 0	
1.009E-03	3.061E-01	10	B324	0 0 0 0 0	
2.291E-03	6.950E-01	20	B179	0 0 0 0 0	
1.084E-03	3.288E-01	20	B300	2 1 1 1 2	
1.085E-03	3.291E-01	20	B324	0 0 0 0 0	
1.084E-03	3.289E-01	20	B324	0 0 0 0 0	
1.381E-03	4.189E-01	30	B324	0 0 0 0 0	
1.381E-03	4.188E-01	30	B324	0 0 0 0 0	
2.307E-03	7.000E-01	rt	M161	0 0 0 0 2	

3164. $C_{13}H_{22}N_2O$
Isonoruron
Urea, 3-[hexahydro-4,7-methanoindan-1(or 2)-yl]-1,1-dimethyl-
Tricuron
BAS 2103H
RN: 28346-65-8 **MP** (°C)**:** 165
MW: 222.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.895E-04	2.200E-01	20	M161	1 0 0 0 2	

3165. $C_{13}H_{22}N_2O$
Noruron
3-(Hexahydro-4,7-methanoindan-5-yl)-1,1-dimethylurea
Norea
RN: 18530-56-8 **MP** (°C)**:** 171
MW: 222.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-04	1.500E-01	20	M061	1 0 0 0 2	
6.747E-04	1.500E-01	25	B200	1 0 0 0 2	
6.747E-04	1.500E-01	ns	G036	0 0 0 0 2	

3166. $C_{13}H_{22}N_2O_3$
5-Ethyl-5-*n*-heptylbarbituric acid
5-Ethyl-5-heptylbarbituric acid
5-Ethyl-5-heptylbarbiturate
RN: 60784-70-5 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.050E-04	1.539E-01	25	M310	2 2 2 2 2	

3167. $C_{13}H_{22}O_3$
Methyl dihydrojasmonate
Hedione
Methyl 3-oxo-2-pentylcyclopentaneacetate
Claigeon
RN: 24851-98-7 **MP** (°C)**:**
MW: 226.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.767E-03	3.998E-01	25	M350	1 0 1 1 1	

3168. $C_{13}H_{24}N_3O_3PS$

Pirimiphos-ethyl
Diethyl *O*-(2-(diethylamino)-6-methyl-4-pyrimidinyl) phosphorothioate
Fernex
Primotec
Solgard
RN: 23505-41-1 **MP** (°C)**:**
MW: 333.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-05	3.967E-03	20	B300	2 1 1 1 2	
<3.00E-06	<1.00E-03	30	M161	1 0 0 0 0	

3169. $C_{13}H_{24}N_4O_3S$

Bupirimate
5-Butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate
Nimrod
RN: 41483-43-6 **MP** (°C)**:** 50.5
MW: 316.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.918E-05	2.189E-02	ns	R427	0 0 0 0 0	
6.953E-05	2.200E-02	rt	M161	0 0 0 0 1	

3170. $C_{13}H_{24}N_6$

1-(Hexamethyleneiminel)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, 6-(hexahydro-1H-azepin-1-yl)-*N,N,N′,N′*-tetramethyl-
RN: 125867-92-7 **MP** (°C)**:**
MW: 264.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-05	5.988E-03	25	B386	0 0 0 0 0	

3171. $C_{13}H_{24}O_4$

Octyl α-acetoxypropionate
Propanoic acid, 2-(acetyloxy)-, octyl ester
RN: 6283-90-5 **MP** (°C)**:**
MW: 244.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.093E-04	1.000E-01	25	R006	2 2 0 1 1	

3172. $C_{13}H_{24}O_4$

1,11-Undecanedicarboxylic acid
1,13-Tridecanedioic acid
Brassylic acid
RN: 505-52-2 **MP** (°C)**:** 111
MW: 244.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.139E-03	1.500E+00	21	B040	1 0 1 1 1	*sic*
1.637E-04	4.000E-02	24	F300	1 0 0 0 0	*sic*

3173. $C_{13}H_{25}NO_3$

Dibutylaceturethane
RN: **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.287E-04	7.999E-02	44	O021	1 2 0 0 0	

3174. $C_{13}H_{26}N_2O_2$

N,N,N′,N′-Tetramethylazelamide
Nonanediamide, *N,N,N′,N′*-tetramethyl-
RN: 13424-87-8 **MP** (°C)**:**
MW: 242.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E+00	9.452E+02	30	D010	1 2 1 1 2	

3175. $C_{13}H_{26}O_2$

n-Tridecanoic acid
Tridecanoic acid
RN: 638-53-9 **MP** (°C)**:** 41.5
MW: 214.35 **BP** (°C)**:** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.797E-05	2.100E-02	0	B136	1 0 2 1 1	
1.540E-04	3.300E-02	20	B136	1 0 2 1 1	
1.539E-04	3.300E-02	20.0	R001	1 1 1 1 1	
1.773E-04	3.800E-02	30	B136	1 0 2 1 1	
1.773E-04	3.800E-02	30.0	R001	1 1 1 1 1	
2.053E-04	4.400E-02	45	B136	1 0 2 1 1	
2.053E-04	4.400E-02	45.0	R001	1 1 1 1 1	
2.519E-04	5.400E-02	60	B136	1 0 2 1 1	
2.519E-04	5.400E-02	60.0	R001	1 1 1 1 1	
9.797E-05	2.100E-02	.0	R001	1 1 1 1 1	

3176. $C_{13}H_{26}O_2$
Methyl laurate
Dodecanoic acid methyl ester
Methyl dodecanoate
RN: 111-82-0 **MP** (°C)**:** 41
MW: 214.35 **BP** (°C)**:** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.05E-05	<4.40E-03	20	M337	2 1 2 2 1	

3177. $C_{13}H_{26}O_3$
n-Octyl β-ethoxypropionate
RN: **MP** (°C)**:**
MW: 230.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.34E-04	<10.00E-02	25	D002	1 2 1 1 0	

3178. $C_{13}H_{26}O_3$
Decyl lactate
2-Hydroxypropionic acid decyl ester
RN: 42175-34-8 **MP** (°C)**:**
MW: 230.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.682E-04	2.000E-01	25	R006	2 2 0 1 0	

3179. $C_{13}H_{26}O_4$
1,3-Dioxolane-4-methanol, 2-[2-(hexyloxy)ethyl]-2-methyl
RN: 124485-63-8 **MP** (°C)**:**
MW: 246.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	3.942E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

3180. $C_{13}H_{28}$
Tridecane
RN: 629-50-5 **MP** (°C)**:** –5.5
MW: 184.37 **BP** (°C)**:** 235.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.170E-09	4.000E-07	25	T423	0 0 0 0 0	

3181. $C_{14}H_4N_2O_2S_2$

Dithianon
1,4-Dithiaanthraquinone-2,3-dinitrile
2,3-Dicyano-1,4-dithiaantraquinone
RN: 3347-22-6 **MP** (°C)**:** 225
MW: 296.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-06	5.000E-04	ns	A305	0 0 0 0 0	
4.677E-07	1.386E-04	ns	R427	0 0 0 0 0	

3182. $C_{14}H_6Cl_2F_4N_2O_2$

Teflubenzuron
Nomolt
RN: 83121-18-0 **MP** (°C)**:**
MW: 381.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.466E-08	9.400E-06	20	M402	0 0 0 0 0	

3183. $C_{14}H_6N_2O_4$

1,4,5,8-Naphthalenediimide
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide
1,4,5,8-Naphthalenetetracarboxylic acid diimide
1,4,5,8-Naphthalenetetracarboxylic diimide
Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone
RN: 5690-24-4 **MP** (°C)**:**
MW: 266.21 **BP** (°C)**:** 656.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		23	B410	2 1 2 2 2	

3184. $C_{14}H_6O_8$

Ellagic acid
2,3,7,8-Tetrahydroxy(1)benzopyrano(5,4,3-cde)(1)benzopyran-5,10-dione
Elagostasine
Benzoaric acid
Alizarine yellow
4,4′,5,5′,6,6′-Hexahydrodiphenic acid 2,6,2′,6′-dilactone
RN: 476-66-4 **MP** (°C)**:** >360
MW: 302.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.210E-05	9.700E-03	37	B438	0 0 0 0 0	

3185. $C_{14}H_7ClO_5S$

1,5-Chloroanthraquinone sulfonic acid
1-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-
RN: **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.033E+00	3.333E+02	18	F047	1 2 1 1 0	

3186. $C_{14}H_7ClO_5S$

1,7-Chloroanthraquinone sulfonic acid
RN: **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3187. $C_{14}H_7ClO_5S$

1,6-Chloroanthraquinone sulfonic acid
2-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-
RN: 300360-23-0 **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3188. $C_{14}H_8Cl_2N_4$

Clofentezine
3,6-bis(2-Chlorophenyl)-1,2,4,5-tetrazine
Apollo
Acaristop
bis(2-Chlorophenyl)-1,2,4,5-tetrazine
Panatac
RN: 74115-24-5 **MP** (°C)**:** 182.3
MW: 303.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-09	2.522E-06	ns	R424	0 0 0 0 0	
8.318E-09	2.522E-06	ns	R427	0 0 0 0 0	

3189. $C_{14}H_8Cl_4$

2,4′-Dichlorodiphenyldichloroethylene
1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethylene
o,p′-DDE
RN: 3424-82-6 **MP** (°C)**:** 76.5
MW: 318.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.402E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 µm

3190. $C_{14}H_8Cl_4$

p,p′-Dichlorodiphenyldichloroethylene
2,2-bis(4-Chlorophenyl)-1,1-dichloroethylene
p,p′-DDE
RN: 72-55-9 **MP** (°C)**:** 89.0
MW: 318.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E-07	5.500E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.258E-07	4.000E-05	20	C053	0 0 0 0 0	
1.258E-07	4.000E-05	20	F071	1 1 2 1 1	
3.773E-07	1.200E-04	25	B083	2 2 1 2 2	particle size 5 µm
3.773E-07	1.200E-04	25	I308	0 0 0 0 0	
4.088E-09	1.300E-06	25	M134	1 2 1 1 1	
4.402E-08	1.400E-05	25	W025	1 0 1 1 1	
7.389E-07	2.350E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.415E-06	4.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
4.717E-09	1.500E-06	ns	M110	0 0 0 0 0	EFG
4.088E-09	1.300E-06	ns	M118	0 1 1 1 1	

3191. $C_{14}H_8O_2$

Anthraquinone
9,10-Anthraquinone
9,10-Dioxoanthracene
Corbit
Morkit
Hoelite
RN: 84-65-1 **MP** (°C)**:** 286
MW: 208.22 **BP** (°C)**:** 377

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-06	1.353E-03	25	E014	2 2 2 1 1	pH 7.3
3.000E-06	6.247E-04	ns	G077	0 0 0 0 1	

3192. $C_{14}H_8O_4$

Alizarin
Alizarine
C.I. Mordant red 11

RN: 72-48-0 **MP** (°C)**:** 290
MW: 240.22 **BP** (°C)**:** 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.123E-03	25	B333	0 0 0 0 0	*sic*
1.664E-03	3.998E-01	rt	D021	0 0 1 1 1	*sic*

3193. $C_{14}H_8O_4$

Quinizarin
1,4-Dihydroxyanthraquinone
C.I. Pigment violet 12

RN: 81-64-1 **MP** (°C)**:** 192
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-07	9.609E-05	25	B333	0 0 0 0 0	
6.000E-05	1.441E-02	98.59	M180	0 0 2 2 0	EFG
9.200E-05	2.210E-02	111.46	M180	0 0 2 2 0	EFG
1.100E-04	2.642E-02	117.47	M180	0 0 2 2 0	EFG
1.800E-04	4.324E-02	123.67	M180	0 0 2 2 0	EFG
2.000E-04	4.804E-02	126.84	M180	0 0 2 2 0	EFG
2.100E-04	5.045E-02	135.00	M180	0 0 2 2 0	EFG
4.900E-04	1.177E-01	141.78	M180	0 0 2 2 0	EFG
7.500E-04	1.802E-01	152.37	M180	0 0 2 2 0	EFG

3194. $C_{14}H_8O_5$

Purpurin
1,2,4-Trihydroxy-anthrachinon

RN: 81-54-9 **MP** (°C)**:**
MW: 256.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.405E-03	25	B333	0 0 0 0 0	

3195. $C_{14}H_8O_6$
Quinalizarin
1,2,5,8-Tetrahydroxyanthraquinone
9,10-Anthracenedione
Alizarine Bordeaux B
Mordant violet 26
RN: 81-61-8 **MP** (°C)**:**
MW: 272.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-06	2.586E-03	25	B333	0 0 0 0 0	

3196. $C_{14}H_8O_8S_2$
Anthraquinone-1,8-disulfonic acid
1,8-Disulfonic acid anthraquinone
Anthrachinon-disulfosaeure-(1,8)
1,8-Anthraquinone disulfonic acid
RN: 82-48-4 **MP** (°C)**:** 293
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3197. $C_{14}H_8O_8S_2$
1,6-Anthraquinone disulfonic acid
Anthraquinone-1,6-disulfonic acid
RN: 14486-58-9 **MP** (°C)**:** 216
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.357E+00	5.000E+02	18	F047	1 2 1 1 0	

3198. $C_{14}H_8O_8S_2$
1,5-Anthraquinone disulfonic acid
Anthraquinone-1,5-disulfonic acid
RN: 252967-17-2 **MP** (°C)**:** 310.0
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3199. $C_{14}H_9ClF_2N_2O_2$

Difluron
Diflubenzuron
TH 6040

RN: 35367-38-5 **MP** (°C)**:** 239
MW: 310.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.437E-07	2.000E-04	20	M161	1 0 0 0 0	
2.865E-07	8.900E-05	20	M402	0 0 0 0 0	
6.437E-07	2.000E-04	20	R303	1 0 0 0 0	
9.656E-07	3.000E-04	24	C105	2 1 2 2 2	
1.609E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
2.570E-07	7.986E-05	ns	R427	0 0 0 0 0	

3200. $C_{14}H_9ClF_3NO_2$

Efavirenz
8-Chloro-5-(2-cyclopropylethynyl)-5-(trifluoromethyl)-4-oxa-2-azabicyclo [4.4.0]deca-7,9,11-trien-3-one

RN: 154598-52-4 **MP** (°C)**:**
MW: 315.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	8.000E-03	ns	A426	0 0 0 0 0	intrinsic
3.168E-05	1.000E-02	ns	K444	0 0 0 0 0	

3201. $C_{14}H_9Cl_2NO_5$

Bifenox
5-(2,4-Dichlorphenoxy)-2-nitro-benzoic acid methyl ester
Modown 4 flowable
Modown

RN: 42576-02-3 **MP** (°C)**:** 85
MW: 342.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.461E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
1.023E-06	3.500E-04	ns	M161	0 0 0 0 1	
1.023E-06	3.501E-04	ns	R427	0 0 0 0 0	

3202. $C_{14}H_9Cl_5$

o,p′-DDT
1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2,2-trichloroethane
2,4′-DDT
2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1,1-trichloroethane
RN: 789-02-6 **MP** (°C)**:** 74.0
MW: 354.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.398E-07	8.500E-05	25	B083	2 2 1 2 1	particle size 5 µm
2.398E-07	8.500E-05	25	I308	0 0 0 0 0	
7.334E-08	2.600E-05	25	W025	1 0 2 2 1	
3.808E-07	1.350E-04	35	B083	2 2 1 2 2	particle size 5 µm
5.642E-07	2.000E-04	45	B083	2 2 1 2 2	particle size 5 µm

3203. $C_{14}H_9Cl_5$

p,p′-DDT
2,2-bis(*p*-Chlorophenyl)-1,1,1-trichloroethane
p,p′-TDEE
RN: 50-29-3 **MP** (°C)**:** 108.5
MW: 354.49 **BP** (°C)**:** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.385E-09	1.200E-06	0	G319	0 0 0 0 0	
1.664E-08	5.900E-06	2	B186	2 0 2 2 2	
4.796E-08	1.700E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.834E-07	6.500E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.800E-07	9.926E-05	18	G054	1 0 1 0 1	
1.410E-08	5.000E-06	20	C111	1 0 0 0 0	
1.410E-08	5.000E-06	20	C113	1 0 2 1 1	
1.128E-07	4.000E-05	20	E048	1 2 1 1 0	
2.172E-08	7.700E-06	20	F303	1 2 1 2 1	
2.172E-08	7.700E-06	20	W319	1 2 1 2 1	
1.552E-08	5.500E-06	24	C311	0 0 0 0 0	EFG
1.523E-08	5.400E-06	24	C313	0 0 0 0 0	
2.821E-09	1.000E-06	24	K069	2 0 0 1 1	
7.079E-08	2.510E-05	24.99	K436	0 0 0 0 0	
3.385E-09	1.200E-06	25	B036	1 1 0 1 1	
3.949E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 µm
7.052E-08	2.500E-05	25	B083	2 2 1 2 1	particle size 5 µm
4.796E-09	1.700E-06	25	B093	2 2 2 2 1	
1.055E-07	3.740E-05	25	B186	2 0 2 2 2	
9.168E-09	3.250E-06	25	F071	1 1 2 1 1	
3.385E-09	1.200E-06	25	M040	1 0 0 1 1	
3.385E-09	1.200E-06	25	M130	1 0 0 0 1	
2.821E-09	1.000E-06	25	P085	0 0 0 0 0	
1.552E-08	5.500E-06	25	W025	1 0 2 2 1	
3.385E-09	1.200E-06	26.70	L095	2 2 1 1 2	

(*continued*)

3203. $C_{14}H_9Cl_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-07	3.700E-05	35	B083	2 2 1 2 1	particle size 5 µm
7.334E-07	2.600E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.269E-07	4.500E-05	37.50	B186	2 0 2 2 2	
1.269E-07	4.500E-05	45	B083	2 2 1 2 1	particle size 5 µm
1.439E-06	5.100E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.552E-08	5.500E-06	ns	C318	0 0 0 0 0	
3.385E-09	1.200E-06	ns	I300	0 0 0 0 1	
4.796E-09	1.700E-06	ns	K138	0 0 0 0 2	
2.821E-09	1.000E-06	ns	M061	0 0 0 0 0	
3.103E-09	1.100E-06	ns	M110	0 0 0 0 0	EFG
5.642E-09	2.000E-06	ns	M138	0 0 0 0 0	
8.745E-09	3.100E-06	ns	M344	0 0 0 0 1	
2.821E-08	1.000E-05	ns	V414	0 0 0 0 0	
2.539E-07	9.000E-05	ns	V414	0 0 0 0 0	

3204. $C_{14}H_9Cl_5O$

Dicofol
4-Chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzenemethanol
4,4′-Dichloro-α-(trichloromethyl)benzhydrol
Acarin
Carbox
Cekudifol

RN: 115-32-2 **MP** (°C)**:** 79
MW: 370.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.563E-06	1.320E-03	25	W025	1 0 2 2 2	

3205. $C_{14}H_9F$

1-Fluoroanthracene

RN: 7651-80-1 **MP** (°C)**:**
MW: 196.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-06	2.600E-04	ns	M344	0 0 0 0 2	

3206. $C_{14}H_9NO_2$
2-Aminoanthraquinone
2-Amino-9,10-anthracenedione
2-Amino-9,10-anthraquinone
Aminoanthraquinone
AAQ
RN: 117-79-3 **MP** (°C)**:** 310
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-07	1.630E-04	25	B333	0 0 0 0 0	

3207. $C_{14}H_9NO_2$
1-Aminoanthraquinone
1-Amino-9,10-anthracenedione
1-Amino-9,10-anthraquinone
RN: 82-45-1 **MP** (°C)**:** 254
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.125E-04	25	B333	0 0 0 0 0	

3208. $C_{14}H_9NO_2$
2-Phenyl-3,1-benzoxazin-4-one
Bentranil
Linarotox
Linurotox
RN: 1022-46-4 **MP** (°C)**:** 123.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.464E-05	5.500E-03	20	M161	1 0 0 0 0	

3209. $C_{14}H_9NO_2S$
4-Benzoyl phenylisothiocyanate
4-Isothiocyanatobenzophenone
RN: 26328-59-6 **MP** (°C)**:**
MW: 255.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	3.574E-03	25	K032	2 2 0 1 1	

3210. $C_{14}H_9NO_3$

1-Amino-4-hydroxyanthraquinone
C.I. Disperse red 15
Disperse red 15
Celliton fast pink B

RN: 116-85-8 **MP** (°C)**:** 208
MW: 239.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.871E-04	25	B333	0 0 0 0 0	
1.129E-05	2.700E-03	60	P313	0 0 0 0 0	average of 2
1.797E-05	4.300E-03	70	P313	0 0 0 0 0	average of 2
2.320E-05	5.550E-03	80	P313	0 0 0 0 0	average of 2
4.828E-05	1.155E-02	90	P313	0 0 0 0 0	average of 2
1.500E-04	3.588E-02	98.59	M180	0 0 2 2 0	EFG
2.500E-04	5.981E-02	111.46	M180	0 0 2 2 0	EFG
3.000E-04	7.177E-02	114.44	M180	0 0 2 2 0	EFG
4.500E-04	1.077E-01	122.10	M180	0 0 2 2 0	EFG
6.000E-04	1.435E-01	126.84	M180	0 0 2 2 0	EFG
6.500E-04	1.555E-01	130.07	M180	0 0 2 2 0	EFG
1.500E-03	3.588E-01	152.37	M180	0 0 2 2 0	EFG

3211. $C_{14}H_{10}$

Phenanthrene
Phenanthracene

RN: 85-01-8 **MP** (°C)**:** 100
MW: 178.24 **BP** (°C)**:** 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.462E-06	2.607E-04	-.7	N053	1 0 0 1 0	EFG
1.970E-06	3.511E-04	4.00	M082	1 1 1 2 2	
1.970E-06	3.511E-04	4.00	M151	2 1 2 2 2	
2.027E-06	3.613E-04	4.04	M183	1 2 1 1 2	
2.265E-06	4.037E-04	4.62	N053	1 0 0 1 0	EFG
2.373E-06	4.230E-04	8.50	M063	2 1 2 2 2	
2.370E-06	4.224E-04	8.50	M082	1 1 1 2 2	
2.370E-06	4.224E-04	8.50	M151	2 1 2 2 2	
2.375E-06	4.233E-04	8.54	M183	1 2 1 1 2	
2.626E-06	4.680E-04	10.00	M063	2 1 2 2 2	
2.630E-06	4.688E-04	10.00	M082	1 1 1 2 2	
2.630E-06	4.688E-04	10.00	M151	2 1 2 2 2	
2.628E-06	4.684E-04	10.04	M183	1 2 1 1 2	
3.055E-06	5.446E-04	10.13	N053	1 0 0 1 0	EFG
2.873E-06	5.120E-04	12.50	M063	2 1 2 2 2	
2.870E-06	5.115E-04	12.50	M082	1 1 1 2 2	
2.870E-06	5.115E-04	12.50	M151	2 1 2 2 2	
2.875E-06	5.124E-04	12.54	M183	1 2 1 1 2	
3.759E-06	6.700E-04	14.20	N053	1 0 0 1 0	EFG
3.372E-06	6.010E-04	15.00	M063	2 1 2 2 2	

(*continued*)

3211. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.370E-06	6.007E-04	15.00	M082	1 1 1 2 2	
3.370E-06	6.007E-04	15.00	M151	2 1 2 2 2	
3.375E-06	6.015E-04	15.04	M183	1 2 1 1 2	
1.500E-05	2.674E-03	20	E025	1 0 2 2 2	
6.200E-06	1.105E-03	20	H306	1 0 1 2 1	
5.061E-06	9.020E-04	20	V416	0 0 0 0 0	
4.420E-06	7.878E-04	20.00	M082	1 1 1 2 2	
4.420E-06	7.878E-04	20.00	M151	2 1 2 2 2	
4.419E-06	7.877E-04	20.04	M183	1 2 1 1 2	
4.578E-06	8.160E-04	21.00	M063	2 1 2 2 2	
4.580E-06	8.163E-04	21.00	M082	1 1 1 2 2	
4.580E-06	8.163E-04	21.00	M151	2 1 2 2 2	
4.582E-06	8.167E-04	21.04	M183	1 2 1 1 2	
7.200E-06	1.283E-03	22	A413	2 0 2 2 1	
5.582E-06	9.950E-04	24.30	M063	2 1 2 2 2	
5.360E-06	9.553E-04	24.30	M082	1 1 1 2 2	
5.360E-06	9.553E-04	24.30	M151	2 1 2 2 2	
5.363E-06	9.558E-04	24.34	M183	1 2 1 1 2	
6.284E-06	1.120E-03	24.60	W003	2 2 2 2 2	average of 2
5.577E-06	9.940E-04	25	A001	1 2 2 2 2	
6.059E-06	1.080E-03	25	B319	2 0 1 2 1	
4.617E-06	8.230E-04	25	D406	1 2 2 2 2	
6.003E-06	1.070E-03	25	E004	2 1 2 2 2	
9.000E-06	1.604E-03	25	K001	2 2 2 2 0	
5.611E-06	1.000E-03	25	L332	1 1 1 1 1	
7.238E-06	1.290E-03	25	M064	1 1 2 2 2	
6.620E-06	1.180E-03	25	M342	1 0 1 1 2	
3.815E-06	6.800E-04	25	P340	0 0 0 0 0	
7.278E-06	1.297E-03	25	T066	1 0 0 0 2	
5.610E-06	9.999E-04	25	W300	2 2 2 2 2	
5.622E-06	1.002E-03	25.00	M151	2 1 1 2 2	
6.800E-06	1.212E-03	25.04	V013	2 2 2 2 2	
5.690E-06	1.014E-03	25.35	N053	1 0 0 1 0	EFG
8.977E-06	1.600E-03	27	D003	1 0 0 1 1	
9.257E-06	1.650E-03	27	D043	2 0 0 0 2	average of 2
7.854E-06	1.400E-03	28.95	N053	1 0 0 1 0	EFG
6.845E-06	1.220E-03	29	M071	2 2 2 2 2	
6.845E-06	1.220E-03	29.00	M151	2 1 1 2 2	
7.165E-06	1.277E-03	29.90	M063	2 1 2 2 2	
7.160E-06	1.276E-03	29.90	M082	1 1 1 2 2	
7.160E-06	1.276E-03	29.90	M151	2 1 2 2 2	
8.360E-06	1.490E-03	29.90	W003	2 2 2 2 2	
6.867E-06	1.224E-03	29.94	M183	1 2 1 1 2	
8.304E-06	1.480E-03	30.30	W003	2 2 2 2 2	average of 2
1.035E-05	1.845E-03	34.53	N053	1 0 0 1 0	EFG
1.375E-05	2.450E-03	38.40	W003	2 2 2 2 2	average of 2
1.440E-05	2.566E-03	40	V416	0 0 0 0 0	
1.274E-05	2.270E-03	40.10	W003	2 2 2 2 2	average of 3
2.171E-05	3.870E-03	47.50	W003	2 2 2 2 2	average of 3

(*continued*)

3211. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.429E-05	4.330E-03	50.10	W003	2 2 2 2 2	average of 3
2.289E-05	4.080E-03	50.20	W003	2 2 2 2 2	average of 3
3.164E-05	5.640E-03	54.70	W003	2 2 2 2 2	average of 3
4.034E-05	7.190E-03	59.20	W003	2 2 2 2 2	average of 3
3.559E-05	6.344E-03	60	V416	0 0 0 0 0	
4.096E-05	7.300E-03	60.50	W003	2 2 2 2 1	average of 3
5.498E-05	9.800E-03	65.10	W003	2 2 2 2 1	average of 3
7.013E-05	1.250E-02	70.70	W003	2 2 2 2 2	average of 3
7.238E-05	1.290E-02	71.90	W003	2 2 2 2 2	
8.528E-05	1.520E-02	73.40	W003	2 2 2 2 2	
7.238E-06	1.290E-03	ns	H123	0 0 0 0 0	
7.238E-06	1.290E-03	ns	K304	0 0 0 0 2	
7.238E-06	1.290E-03	ns	M344	0 0 0 0 2	
1.500E-05	2.674E-03	ns	W005	0 0 1 2 1	

3212. $C_{14}H_{10}$

Anthracene
Paranaphthalene
Anthracin
Green oil
Anthraxcene

RN: 120-12-7 **MP** (°C)**:** 218
MW: 178.24 **BP** (°C)**:** 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.125E-08	1.270E-05	5.20	M063	2 1 2 2 2	
7.100E-08	1.265E-05	5.20	M082	1 1 1 2 1	
7.100E-08	1.265E-05	5.20	M151	2 1 2 2 1	
7.133E-08	1.271E-05	5.24	M183	1 2 1 1 2	
9.818E-08	1.750E-05	10.00	M063	2 1 2 2 2	
9.800E-08	1.747E-05	10.00	M082	1 1 1 2 1	
9.800E-08	1.747E-05	10.00	M151	2 1 2 2 1	
9.828E-08	1.752E-05	10.04	M183	1 2 1 1 2	
9.094E-08	1.621E-05	9.74	M183	1 2 1 1 2	
1.246E-07	2.220E-05	14.10	M063	2 1 2 2 2	
1.250E-07	2.228E-05	14.10	M082	1 1 1 2 2	
1.250E-07	2.228E-05	14.10	M151	2 1 2 2 2	
1.247E-07	2.223E-05	14.14	M183	1 2 1 1 2	
1.212E-07	2.160E-05	15	B385	0 0 0 0 0	
1.409E-07	2.512E-05	16.64	M183	1 2 1 1 2	
1.633E-07	2.910E-05	18.30	M063	2 1 2 2 2	
1.630E-07	2.905E-05	18.30	M082	1 1 1 2 2	
1.630E-07	2.905E-05	18.30	M151	2 1 2 2 2	
1.634E-07	2.912E-05	18.34	M183	1 2 1 1 2	
2.400E-07	4.278E-05	20	E009	1 0 0 0 1	
2.240E-07	3.992E-05	20	E025	1 0 2 2 2	
1.851E-07	3.300E-05	20	H300	1 1 2 2 1	

(*continued*)

3212. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.087E-07	3.720E-05	22.40	M063	2 1 2 2 2	
2.090E-07	3.725E-05	22.40	M082	1 1 1 2 2	
2.090E-07	3.725E-05	22.40	M151	2 1 2 2 2	
2.089E-07	3.723E-05	22.44	M183	1 2 1 1 2	
2.974E-07	5.300E-05	22.5	G301	0 0 0 0 0	
3.927E-07	7.000E-05	23	P332	0 0 0 0 0	
3.927E-07	7.000E-05	23	P339	0 0 0 0 0	
2.123E-07	3.784E-05	23.24	M183	1 2 1 1 2	
2.435E-07	4.340E-05	24.60	M063	2 1 2 2 2	
2.440E-07	4.349E-05	24.60	M082	1 1 1 2 2	
2.440E-07	4.349E-05	24.60	M151	2 1 2 2 2	
2.437E-07	4.344E-05	24.64	M183	1 2 1 1 2	
2.500E-07	4.456E-05	25	A325	2 1 2 2 1	
2.188E-07	3.900E-05	25	B319	2 0 1 2 1	average of 2
2.174E-07	3.875E-05	25	B385	0 0 0 0 0	
5.218E-07	9.300E-05	25	D406	1 2 2 2 2	
4.470E-07	7.967E-05	25	K001	2 2 2 2 2	
3.800E-07	6.773E-05	25	K123	1 0 2 2 1	
4.152E-07	7.400E-05	25	L301	1 1 2 2 2	
3.927E-07	7.000E-05	25	L332	1 1 1 1 2	
4.096E-07	7.300E-05	25	M064	1 1 2 2 1	
4.100E-06	7.308E-04	25	M342	1 0 1 1 2	
1.683E-07	3.000E-05	25	S227	1 2 1 1 1	
4.211E-07	7.506E-05	25	T066	1 0 0 0 2	
2.500E-07	4.456E-05	25	W300	2 2 2 2 2	
2.502E-07	4.460E-05	25.00	M151	2 1 1 2 2	
4.208E-07	7.500E-05	27	D003	1 0 0 1 1	
3.125E-07	5.570E-05	28.70	M063	2 1 2 2 2	
3.130E-07	5.579E-05	28.70	M082	1 1 1 2 2	
3.130E-07	5.579E-05	28.70	M151	2 1 2 2 2	
3.128E-07	5.575E-05	28.74	M183	1 2 1 1 2	
3.198E-07	5.700E-05	29	M071	2 2 2 2 2	
3.198E-07	5.700E-05	29.00	M151	2 1 1 2 2	
3.212E-07	5.724E-05	29.34	M183	1 2 1 1 2	
3.512E-07	6.260E-05	35	B385	0 0 0 0 0	
6.845E-07	1.220E-04	35.40	W003	2 2 2 2 2	average of 3
8.416E-07	1.500E-04	39.30	W003	2 2 2 2 2	average of 3
1.167E-06	2.080E-04	44.70	W003	2 2 2 2 2	average of 3
1.565E-06	2.790E-04	47.50	W003	2 2 2 2 2	
1.683E-06	3.000E-04	50.10	W003	2 2 2 2 2	average of 3
2.211E-06	3.940E-04	54.70	W003	2 2 2 2 2	average of 3
2.794E-06	4.980E-04	59.20	W003	2 2 2 2 2	average of 3
3.703E-06	6.600E-04	64.50	W003	2 2 2 2 1	average of 3
3.703E-06	6.600E-04	65.10	W003	2 2 2 2 1	average of 3
5.162E-06	9.200E-04	69.80	W003	2 2 2 2 1	
5.274E-06	9.400E-04	70.70	W003	2 2 2 2 1	average of 3
5.106E-06	9.100E-04	71.90	W003	2 2 2 2 2	
6.677E-06	1.190E-03	74.70	W003	2 2 2 2 2	average of 3
2.356E-07	4.200E-05	ns	H123	0 0 0 0 0	

(*continued*)

3212. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	3.208E-05	ns	H306	1 0 1 2 1	
4.096E-07	7.300E-05	ns	K304	0 0 0 0 1	
4.096E-07	7.300E-05	ns	M344	0 0 0 0 2	
5.000E-07	8.912E-05	ns	W005	0 0 1 2 0	

3213. $C_{14}H_{10}Cl_2O_3$

Fenclofenac
Benzeneacetic acid, 2-(2,4-dichlorophenoxy)-
RX 67408

RN: 34645-84-6 **MP** (°C)**:** 136
MW: 297.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.840E-05	8.439E-03	25	C314	0 0 0 0 0	
2.827E-05	8.400E-03	25	C314	0 0 0 0 0	

3214. $C_{14}H_{10}Cl_4$

DDD
1,1-Dichloro-2,2-bis(*p*-chlorophenyl)ethane
p,p′-TDE
Dichlorodiphenyldichloroethane

RN: 72-54-8 **MP** (°C)**:** 109.5
MW: 320.05 **BP** (°C)**:** 193

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.812E-07	9.000E-05	25	B083	2 2 1 2 1	particle size 5 µm
6.249E-08	2.000E-05	25	W025	1 0 2 2 1	
4.687E-07	1.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
7.499E-07	2.400E-04	45	B083	2 2 1 2 2	particle size 5 µm
9.374E-09	3.000E-06	ns	M110	0 0 0 0 0	EFG

3215. $C_{14}H_{10}Cl_4$

1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane
o,p′-DDD

RN: 53-19-0 **MP** (°C)**:** 76
MW: 320.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.875E-07	6.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
3.125E-07	1.000E-04	25	B083	2 2 1 2 2	particle size 5 µm
8.749E-07	2.800E-04	35	B083	2 2 1 2 2	particle size 5 µm
9.842E-07	3.150E-04	45	B083	2 2 1 2 2	particle size 5 µm

3216. $C_{14}H_{10}F_3NO_2$

Flufenamic acid
N-(α,α,α-Trifluoro-*m*-tolyl)anthranilic acid
N-(3-Trifluoromethylphenyl)anthranilic acid
RN: 530-78-9 **MP** (°C)**:** 132–135
MW: 281.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-06	1.094E-03	25	G085	2 0 0 0 0	EFG
4.000E-05	1.125E-02	25	I007	1 2 2 2 0	EFG
1.031E-04	2.900E-02	30	D015	2 0 1 1 0	EFG
6.670E-06	1.876E-03	35	G085	2 0 0 0 0	EFG
6.200E-04	1.744E-01	35	H091	1 2 2 2 1	*sic*
2.133E-04	6.000E-02	37	D015	2 0 1 1 0	EFG
3.556E-05	1.000E-02	rt	H302	0 0 2 1 2	intrinsic

3217. $C_{14}H_{10}N_2O_2$

C.I. Disperse violet 1
1,4-Diamino-9,10-anthraquinone
Acetate red violet R
Acetoquinone light heliotrope NL
Supracet brilliant violet 3R
Violet 14447
RN: 128-95-0 **MP** (°C)**:** 275
MW: 238.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-07	2.287E-04	25	B333	0 0 0 0 0	

3218. $C_{14}H_{10}N_2O_6$

Dipentum
Olsalazine
RN: 15722-48-2 **MP** (°C)**:**
MW: 302.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.149E-05	25	D311	0 0 0 0 0	0.1M NaCl

3219. $C_{14}H_{10}O$

2-Anthranol
2-Anthrol
RN: 613-14-9 **MP** (°C)**:**
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-04	9.167E-02	25	L085	1 2 0 1 2	

3220. $C_{14}H_{10}O$

1-Anthranol
1-Anthrol
Anthranol

RN: 529-86-2 **MP** (°C)**:** 152
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.593E-02	25	L085	1 2 0 1 2	

3221. $C_{14}H_{10}O_3$

Diphenyleneglycollic acid

RN: **MP** (°C)**:**
MW: 226.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.082E-02	2.448E+00	25	K040	1 0 2 1 2	

3222. $C_{14}H_{10}O_4$

Diphenic acid
1,1′-Biphenyl-2,2′-dicarboxylic acid
2,2′-Biphenyldicarboxylic acid

RN: 482-05-3 **MP** (°C)**:** 228
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	1.260E+00	25	K040	1 0 2 1 2	

3223. $C_{14}H_{10}O_4$

Benzoyl peroxide
Benzoyl-peroxid

RN: 94-36-0 **MP** (°C)**:** 105
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-07	1.550E-04	rt	C342	0 0 0 0 0	

3224. $C_{14}H_{10}O_5$

Gentisin
9H-Xanthen-9-one, 1,7-dihydroxy-3-methoxy-
Gentianic acid
Gentianin

RN: 437-50-3 **MP** (°C)**:** 266.5
MW: 258.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-03	3.000E-01	16	F300	1 0 0 0 2	

3225. $C_{14}H_{10}O_9$

Digallic acid
m-Digallic acid
m-Digallussaeure

RN: 536-08-3 **MP** (°C)**:**
MW: 322.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.552E-03	5.000E-01	25	F300	1 0 0 0 0	
5.896E-02	1.900E+01	100	F300	1 0 0 0 1	

3226. $C_{14}H_{11}ClNO_2$

7-Chloro-5,11-dihydrodibenz[b,e][1,4]oxazepine-5-carboxamide

RN: **MP** (°C)**:**
MW: 260.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.534E-04	4.000E-02	37	G020	1 0 0 0 1	

3227. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′chloro-2-hydroxy-5-nitrobenzanilide
Benzamide, *N*-(3-chloro-2-methyphenyl)-2-hydroxy-5-nitro-

RN: 213460-66-3 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-05	3.379E-03	25	D400	2 0 0 1 2	

3228. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-5′-chloro-2-hydroxy-5-nitrobenzanilide
Benzamide, *N*-(5-chloro-2-methylphenyl)-2-hydroxy-5-nitro-
RN: 213460-65-2 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.534E-06	2.311E-03	25	D400	2 0 0 1 2	

3229. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′-chloro-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(3-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 73544-88-4 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:** 324.7–408.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3230. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′-chloro-2-hydroxy-3nitrobenzanilide
Benzamide, *N*-(5-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 213460-62-9 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3231. $C_{14}H_{11}ClN_2O_4S$

Chlorthalidone
2-Chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isoindol-1-yl)benzenesulfonamide
Hygroton
Thalitone
Chlortalidone
RN: 77-36-1 **MP** (°C)**:**
MW: 338.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.542E-04	1.200E-01	25	P312	0 0 0 0 0	
4.510E-04	1.528E-01	ns	I304	0 0 0 0 0	

3232. $C_{14}H_{11}Cl_2NO_2$

Diclofenac
2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid
RN: 15307-86-5 **MP** (°C)**:** 157
MW: 296.16 **BP** (°C)**:** 412

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.317E-06	1.278E-03	30	P438	0 0 0 0 0	pH 2.0
1.182E-05	3.500E-03	32	C411	2 1 1 2 1	
4.478E-06	1.326E-03	33	P438	0 0 0 0 0	pH 2.0
5.117E-06	1.515E-03	37	P438	0 0 0 0 0	pH 2.0
5.389E-06	1.596E-03	39.5	P438	0 0 0 0 0	pH 2.0
5.822E-06	1.724E-03	42	P438	0 0 0 0 0	pH 2.0

3233. $C_{14}H_{11}Cl_3O_2$

2,2-bis(-*p*-Hydroxyphenyl)-1,1,1-trichloroethylene
Hydroxychlor
p,p′-Hydroxy-DDT
RN: 2971-36-0 **MP** (°C)**:** 194
MW: 317.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-04	7.600E-02	ns	K117	0 1 2 1 1	

3234. $C_{14}H_{11}FN_2O_5$

1-Acetoxymethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Acetoxymethyl-3-benzoyl-5-fluorouracil
RN: 97096-67-8 **MP** (°C)**:** 127–128
MW: 306.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.400E-01	22	B321	0 0 0 0 0	pH 4.0

3235. $C_{14}H_{11}N$

2-Aminoanthracene
2-Anthrylamine
β-Aminoanthracene
2-Anthracenamine
2-Anthramine
Anthracene amine
RN: 613-13-8 **MP** (°C)**:** 238
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-06	1.300E-03	24	H106	1 0 2 2 2	
6.727E-09	1.300E-06	ns	M349	0 2 1 1 2	

3236. $C_{14}H_{11}N$
Acetonitrile, diphenyl-
Diphenatrile
RN: 86-29-3 **MP** (°C)**:** 74
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-03	2.200E-01	ns	B185	0 0 0 0 0	

3237. $C_{14}H_{11}NO_2$
N-Benzoylbenzamide
Dibenzamid
RN: 614-28-8 **MP** (°C)**:** 152
MW: 225.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.327E-03	1.200E+00	15	F300	1 0 0 0 1	

3238. $C_{14}H_{11}N_3O_2$
Salicylolhydrazone of picolinealdehyde
RN: **MP** (°C)**:**
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.897E-04	2.000E-01	ns	G089	0 1 2 0 1	

3239. $C_{14}H_{12}$
1-Methylfluorene
1-Methyl-9H-fluorene
RN: 1730-37-6 **MP** (°C)**:** 87
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-06	1.090E-03	25	B319	2 0 1 2 2	
6.060E-06	1.092E-03	25	M342	1 0 1 1 2	

3240. $C_{14}H_{12}$
1,1-Diphenylethene
1,1-Diphenylethylene
RN: 530-48-3 **MP** (°C)**:** 8.2
MW: 180.25 **BP** (°C)**:** 277

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.662E-05	6.600E-03	25	A002	1 0 1 1 1	

3241. $C_{14}H_{12}$

9,10-Dihydroanthracene

RN: 613-31-0 **MP** (°C)**:** 104–107
MW: 180.25 **BP** (°C)**:** 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.578E-06	4.646E-04	4.96	R423	0 0 0 0 0	
2.622E-06	4.727E-04	5.85	R423	0 0 0 0 0	
2.917E-06	5.257E-04	7.95	R423	0 0 0 0 0	
3.317E-06	5.978E-04	10.95	R423	0 0 0 0 0	
3.556E-06	6.409E-04	12.05	R423	0 0 0 0 0	
4.261E-06	7.681E-04	14.95	R423	0 0 0 0 0	
4.961E-06	8.942E-04	18.00	R423	0 0 0 0 0	
5.811E-06	1.047E-03	20.96	R423	0 0 0 0 0	
7.389E-06	1.332E-03	24.59	R423	0 0 0 0 0	
8.011E-06	1.444E-03	26.59	R423	0 0 0 0 0	
9.400E-06	1.694E-03	29.05	R423	0 0 0 0 0	
1.114E-05	2.009E-03	32.66	R423	0 0 0 0 0	
1.288E-05	2.321E-03	36.28	R423	0 0 0 0 0	
1.498E-05	2.701E-03	40.01	R423	0 0 0 0 0	

3242. $C_{14}H_{12}$

trans-Stilbene
trans-Diphenylethylene
1,2-Diphenylethene
trans-1,2-Diphenylethylene
trans-α, β-Diphenylethylene
Toluylene

RN: 103-30-0 **MP** (°C)**:** 124
MW: 180.25 **BP** (°C)**:** 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.609E-06	2.900E-04	25	A002	1 0 1 1 1	

3243. $C_{14}H_{12}F_3NO_4S_2$

Perfluidone
Methyl-4-(phenylsulfonyl)trifluoromethanesulfonanilide
1,1,1-Trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide
Destun
MBR 8251
Trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide

RN: 37924-13-3 **MP** (°C)**:** 143
MW: 379.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.582E-04	6.000E-02	22	G306	1 0 0 0 1	
1.582E-04	6.000E-02	22	M161	1 0 0 0 1	

3244. $C_{14}H_{12}N_2O_4$
4′-Methyl-2-hydroxy-5-nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(4-methylphenyl)--nitro-
RN: 68507-96-0 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-05	3.846E-03	25	D400	2 0 0 1 2	

3245. $C_{14}H_{12}N_2O_4$
4′-Methyl-2-hydroxy-3-nitrobenzanilide
Benzamide,2-hydroxy-*N*-(4-methylpheyl)-3-nitro-
RN: 68507-90-4 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:** 305.7–389.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E-05	8.356E-03	25	D400	2 0 0 1 2	

3246. $C_{14}H_{12}N_2O_4$
2′-Methyl-2-hydroxy-3-nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(2-methylphenyl)-3-nitro-
RN: 68507-89-1 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:** 302–384.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.818E-05	7.673E-03	25	D400	2 0 0 1 2	

3247. $C_{14}H_{12}N_2O_5$
4′-Methoxy-2-hydroxy-5nitrobenzanilide
p-Salicylanisidide, 5-nitro-
Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-5-nitro-
RN: 68507-94-8 **MP** (°C)**:**
MW: 288.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-05	5.556E-03	25	D400	2 0 0 1 2	

3248. $C_{14}H_{12}N_2O_5$
4′-Methoxy-2-hydroxy-3nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-3-nitro-
RN: 68507-88-0 **MP** (°C)**:**
MW: 288.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.532E-05	1.018E-02	25	D400	2 0 0 1 2	

3249. $C_{14}H_{12}N_2S$

2-(4-Aminophenyl)-6-methyl-benzothiazole
Dehydrothio-*N*-toluidin
Dehydrothio-*N*-toluidine

RN: 92-36-4 **MP** (°C)**:** 194.8
MW: 240.33 **BP** (°C)**:** 434

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.080E-04	5.000E-02	100	F300	1 0 0 0 0	

3250. $C_{14}H_{12}N_4O_2$

C.I. Disperse blue 1
9,10-Anthracenedione, 1,4,5,8-tetraamino-

RN: 2475-45-8 **MP** (°C)**:** 332
MW: 268.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.683E-05	25	B333	0 0 0 0 0	

3251. $C_{14}H_{12}O_2$

4-Biphenylacetic acid
Felbinac

RN: 5728-52-9 **MP** (°C)**:**
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.927E-02	25	P344	0 0 0 0 0	EFG

3252. $C_{14}H_{12}O_2$

Benzoin
2-Hydroxy-1,2-diphenylethanone
Benzoylphenylcarbinol
2-Hydroxy-2-phenylacetophenone
Hydroxy-2-phenyl acetophenone

RN: 579-44-2 **MP** (°C)**:** 137
MW: 212.25 **BP** (°C)**:** 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	3.000E-01	25	F300	1 0 0 0 0	
1.413E-03	2.999E-01	rt	D021	0 0 1 1 0	

3253. $C_{14}H_{12}O_2$

Benzyl benzoate
Ascabin
Scabagen
Benzoic acid phenylmethyl ester
Benylate
Phenylmethyl benzoate

RN: 120-51-4 **MP** (°C)**:** 19
MW: 212.25 **BP** (°C)**:** 323

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.225E-04	2.600E-02	15	H069	1 0 1 1 1	
6.960E-03	1.477E+00	30	M444	0 0 0 0 0	
7.020E-03	1.490E+00	40	M444	0 0 0 0 0	
7.150E-03	1.518E+00	50	M444	0 0 0 0 0	
7.230E-03	1.535E+00	60	M444	0 0 0 0 0	

3254. $C_{14}H_{12}O_2$

Diphenylacetic acid
Diphenyl-essigsaeure

RN: 117-34-0 **MP** (°C)**:** 148
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.274E-01	25	K040	1 0 2 1 2	

3255. $C_{14}H_{12}O_3$

Benzilic acid
2,2-Diphenyl-2-hydroxyacetic acid
Diphenylglycolic acid
Benzeneacetic acid, α-hydroxy-α-phenyl-
2-Hydroxy-2,2-diphenylethanoic acid

RN: 76-93-7 **MP** (°C)**:** 150
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-03	1.755E+00	25	K040	1 0 2 1 2	
6.190E-03	1.413E+00	25	L050	2 0 1 2 2	

3256. $C_{14}H_{12}O_3$

Benzylparaben
Benzyl 4-hydroxybenzoate
Phenylmethyl ester

RN: 94-18-8 **MP** (°C)**:**
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.200E-02	25	P013	0 0 0 0 0	

3257. $C_{14}H_{12}O_5$

Khellin
Amicardine

RN: 82-02-0 **MP** (°C)**:** 154.5
MW: 260.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-01	2.472E+02	25	E312	0 0 0 0 0	EFG, *sic*
1.153E-04	3.000E-02	25	J028	1 2 0 2 0	
7.000E-04	1.822E-01	30	E012	1 2 1 1 0	
1.300E-03	3.383E-01	42	E012	1 2 1 1 0	

3258. $C_{14}H_{13}ClN_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-

RN: 133627-12-0 **MP** (°C)**:**
MW: 288.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.691E-05	2.221E-02	ns	M381	0 1 1 1 2	pH 7.0

3259. $C_{14}H_{13}NO_6$

Benzoic acid, 2-(acetyloxy)-, (2,5-dioxo-1-pyrrolidinyl)methyl ester
Salicylic acid acetate, ester with *N*-(hydroxymethyl)succinimide

RN: 32620-72-7 **MP** (°C)**:** 117.5
MW: 291.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.717E-03	5.000E-01	21	N335	0 0 0 0 0	

3260. $C_{14}H_{13}N_2$
4,7-Dimethyl-1,10-phenanthroline
4,7-Dimethyl-*o*-phenanthroline
RN: 3248-05-3 **MP** (°C)**:** 193
MW: 209.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.239E-02	25.04	B094	1 2 1 2 2	

3261. $C_{14}H_{13}N_3O_2$
Pyrido[2,3-b][1,5]benzoxazepin-5(6H)-one, 3-amino-6,9-dimethyl-
RN: 134894-45-4 **MP** (°C)**:**
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.057E-04	2.312E-01	ns	M381	0 1 1 1 2	pH 7.0

3262. $C_{14}H_{13}N_3O_4S_2$
Meloxicam
RN: 71125-38-7 **MP** (°C)**:**
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	2.284E-02	25	C434	0 0 0 0 0	pH 6.0
3.415E-05	1.200E-02	25	S415	0 0 0 0 0	
9.500E-05	3.338E-02	30	C434	0 0 0 0 0	pH 6.0
1.550E-05	5.447E-03	37	C434	0 0 0 0 0	pH 6.0
3.699E-06	1.300E-03	37	Y421	0 0 0 0 0	
2.800E-05	9.839E-03	45	C434	0 0 0 0 0	pH 6.0

3263. $C_{14}H_{14}$
4,4′-Dimethylbiphenyl
4,4′-Dimethyl-1,1′-biphenyl
p,p′-Bitoluene
RN: 613-33-2 **MP** (°C)**:** 125.0
MW: 182.27 **BP** (°C)**:** 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.770E-07	6.871E-05	4.0	D330	2 2 1 2 2	
9.590E-07	1.748E-04	25.0	D330	2 2 1 2 2	
2.420E-06	4.411E-04	40.0	D330	2 2 1 2 2	

3264. $C_{14}H_{14}$

Bibenzyl
1,2-Diphenylethane
Benzene, 1,1′-(1,2-ethanediyl)*bis*-
RN: 103-29-7 **MP** (°C)**:** 52.0
MW: 182.27 **BP** (°C)**:** 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.359E-05	4.300E-03	25	A002	1 0 1 1 1	

3265. $C_{14}H_{14}NO_4PS$

EPN
Ethyl *O*-(*p*-nitrophenyl) phenylphosphonothionate
O-Ethyl *O*-*p*-nitrophenyl benzenephosphonothioate
Ethyl *O*-(*p*-nitrophenyl) benzenethiophosphonate
RN: 2104-64-5 **MP** (°C)**:** 36
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-06	3.113E-03	22	K137	1 1 2 1 0	

3266. $C_{14}H_{14}N_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl
RN: 132312-85-7 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-03	6.100E-01	ns	M381	0 1 1 1 2	pH 7.0

3267. $C_{14}H_{14}N_4O_2$

Dis. A. 7
RN: 2491-74-9 **MP** (°C)**:** 236
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-09	5.406E-07	25	B333	0 0 0 0 0	

3268. $C_{14}H_{14}N_4O_2$

Dye II
4-[[(4-Dimethylamino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-07	2.108E-04	84.10	B198	1 2 1 1 1	
2.040E-06	5.514E-04	97.40	B198	1 2 1 1 2	

3269. $C_{14}H_{14}N_4O_4$

β,γ-Dihydroxypropyltheophylline

RN: 180262-60-6 **MP** (°C)**:**

MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.007E-01	9.091E+01	ns	J025	0 0 0 0 1	

3270. $C_{14}H_{14}N_4S$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepine-6-thione, 11-ethyl-5,11-dihydro-5-methyl

RN: 134698-27-4 **MP** (°C)**:**

MW: 270.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-05	6.280E-03	ns	M381	0 1 1 1 2	pH 7.0

3271. $C_{14}H_{14}O$

6-Benzyl-*m*-cresol

Phenol, 5-methyl-2-(phenylmethyl)-

RN: 30091-04-4 **MP** (°C)**:**

MW: 198.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-04	2.857E-02	25	L021	1 0 0 0 0	

3272. $C_{14}H_{14}O$

DL-1,2-Diphenylethanol

DL-1,2-Diphenyl-aethanol

RN: 614-29-9 **MP** (°C)**:** 67

MW: 198.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-03	6.000E-01	100	F300	1 0 0 0 0	

3273. $C_{14}H_{14}O_2$

DL-Hydrobenzoin

Hydrobenzoin

RN: 27134-24-3 **MP** (°C)**:** 139

MW: 214.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E-02	2.500E+00	15	F300	1 0 0 0 1	
8.867E-03	1.900E+00	15	F300	1 0 0 0 1	
6.021E-02	1.290E+01	100	F300	1 0 0 0 2	

3274. $C_{14}H_{14}O_3$

Pindone
2-Pivaloylindandione-1,3
RN: 83-26-1 **MP** (°C)**:** 109
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-05	1.800E-02	25	M061	1 0 0 0 1	
7.817E-05	1.800E-02	25	M161	1 0 0 0 1	

3275. $C_{14}H_{14}O_3$

Naproxen
6-Methoxy-α-methyl-2-naphthaleneacetic acid
(*S*)-6-Methoxy-α-methyl-2-naphthaleneacetic acid
Laraflex
RN: 22204-53-1 **MP** (°C)**:** 155.3
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-05	9.924E-03	5	F306	1 0 1 2 2	intrinsic
6.948E-05	1.600E-02	21	B331	1 2 2 1 2	pH 7.4
6.080E-05	1.400E-02	25	A408	2 0 1 2 0	int
6.905E-05	1.590E-02	25	A427	0 0 0 0 0	
6.905E-05	1.590E-02	25	C059	1 2 1 1 2	
6.900E-05	1.589E-02	25	F306	1 0 1 2 2	intrinsic
1.146E-04	2.639E-02	37	F306	1 0 1 2 2	intrinsic
2.171E-05	5.000E-03	37	Y421	0 0 0 0 0	
5.211E-04	1.200E-01	amb	L434	0 0 0 0 0	
5.646E-05	1.300E-02	rt	H302	0 0 2 1 2	intrinsic

3276. $C_{14}H_{14}O_3S$

o-Cresyl-*p*-toluene sulfonate
2-Methylphenyl tosylate
o-Tolyl tosylate
2-Tolyl tosylate
RN: 599-75-7 **MP** (°C)**:**
MW: 262.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.144E-04	3.000E-02	ns	F014	0 0 0 0 0	

3277. $C_{14}H_{14}O_4$

Diallyl *m*-phthalate

RN: **MP** (°C)**:**
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-04	4.900E-02	25	S417	0 0 0 0 0	

3278. $C_{14}H_{14}O_4$

Diallyl phthalate
Di-2-propenyl phthalate

RN: 131-17-9 **MP** (°C)**:** –70
MW: 246.27 **BP** (°C)**:** 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.06E-04	<10.00E-02	20	F070	1 0 0 0 1	
7.390E-04	1.820E-01	20	L300	2 1 0 2 2	
7.413E-04	1.826E-01	ns	S460	0 0 0 0 0	

3279. $C_{14}H_{15}N$

p-Aminostilbene
4-Aminostilbene

RN: 834-24-2 **MP** (°C)**:**
MW: 197.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	5.000E-03	rt	N015	0 0 2 2 0	

3280. $C_{14}H_{15}NO_5$

L-Proline, 1-[(benzoyloxy)acetyl]-

RN: 115178-75-1 **MP** (°C)**:** 72.5
MW: 277.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-02	7.100E+00	22	N317	1 1 2 1 2	

3281. $C_{14}H_{15}N_3$

o-Aminoazotoluene
2-Amino-5-azotoluene

RN: 97-56-3 **MP** (°C)**:** 101
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.107E-05	7.000E-03	37	H120	1 1 1 1 1	normal saline

3282. $C_{14}H_{15}N_3$

p-Dimethylaminoazobenzene
4-Dimethylaminoazobenzol
Dimethylaminoazobenzene
Methylgelb
C. I. Solvent yellow 2

RN: 60-11-7 **MP** (°C)**:** 116
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.877E-04	2.000E-01	20	F300	1 0 0 0 0	
6.214E-06	1.400E-03	20	J027	1 0 0 0 1	
1.700E-06	3.830E-04	25	B333	0 0 0 0 0	*sic*
1.775E-06	4.000E-04	30	R430	0 0 0 0 0	
7.101E-04	1.600E-01	rt	D021	0 0 1 1 1	*sic*

3283. $C_{14}H_{15}N_3O_3S$

Gly-dapsone
Acetamide, 2-amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]

RN: 160349-02-0 **MP** (°C)**:**
MW: 305.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.849E-03	8.700E-01	25	P351	0 0 0 0 0	pH 7.4
>4.91E-02	>1.50E+01	25	P351	0 0 0 0 0	

3284. $C_{14}H_{15}N_5O_5$

9-(2-*O*-Butyryl-β-D-arabinofuranosyl)adenine
9H-Purin-6-amine, 9-[3,5-*bis*-*O*-[(1,1-dimethylethyl)dimethylsilyl]-2-*O*-(1-oxobutyl)-β-D-arabinofuranosyl]-

RN: 87970-05-6 **MP** (°C)**:**
MW: 333.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-04	3.410E-02	37	B306	1 2 0 1 2	pH 7.3

3285. $C_{14}H_{15}N_5O_6S$

Metasulfron-methyl
Metsulfuron methyl ester
Allie
Escort
DPX-T6376
Ally

RN: 74223-64-6 **MP** (°C)**:** 158
MW: 381.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-05	2.700E-02	ns	R427	0 0 0 0 0	

3286. $C_{14}H_{15}O_2PS_2$

Edifenphos

RN: 17109-49-8 **MP** (°C)**:**
MW: 310.38 **BP** (°C)**:** 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.803E-04	5.596E-02	ns	S460	0 0 0 0 0	

3287. $C_{14}H_{16}ClN_3O_2$

Triadimefon

1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone

Triamefon

Bayleton

RN: 43121-43-3 **MP** (°C)**:** 82.3
MW: 293.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.851E-04	2.600E-01	20	M161	1 0 0 0 2	

3288. $C_{14}H_{16}ClO_5PS$

Coumaphos

O,O-Diethyl *O*-(3-chloro-4-methylcoumarinyl-7) thiophosphate

RN: 56-72-4 **MP** (°C)**:** 91
MW: 362.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.135E-06	1.500E-03	20	M061	1 0 0 0 1	
4.169E-06	1.512E-03	ns	R427	0 0 0 0 0	

3289. $C_{14}H_{16}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid cyclohexyl ester

Cyclohexyl 2,4-dichlorophenoxyacetate

RN: 65267-97-2 **MP** (°C)**:**
MW: 303.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.811E-05	5.492E-03	ns	M120	0 0 1 1 2	

3290. $C_{14}H_{16}FN_3O_3$

2,5-Diaziridinyl-3-floro-6-morpholino-1,4-benzoquinone

2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1-aziridinyl)-3-fluoro-6-(4-morpholinyl)-

RN: 59886-45-2 **MP** (°C)**:** 157
MW: 293.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-03	2.000E+00	rt	C317	0 0 0 0 0	

3291. $C_{14}H_{16}F_3N_3O_4$

Profluralin
N-(Cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine
Pregard
Tolban
ER-5461

RN: 26399-36-0 **MP** (°C)**:** 32
MW: 347.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E-07	1.000E-04	20	E048	1 2 1 1 0	
2.879E-07	1.000E-04	20	M161	1 0 0 0 0	
2.879E-07	1.000E-04	27	K315	1 0 0 0 1	

3292. $C_{14}H_{16}N_2$

o-Tolidine
3,3′-Dimethylbenzidine

RN: 119-93-7 **MP** (°C)**:** 130.0
MW: 212.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E-03	1.300E+00	25	B068	2 0 1 1 1	

3293. $C_{14}H_{16}N_2O_2$

3,3′-Dimethoxybenzidine
o-Dianisidine
Dianisidine

RN: 119-90-4 **MP** (°C)**:** 137
MW: 244.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.456E-04	6.000E-02	25	B068	2 0 1 1 0	

3294. $C_{14}H_{16}N_2O_4$

2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-

RN: 116482-82-7 **MP** (°C)**:** 194.5
MW: 276.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	N317	1 1 2 1 2	

3295. $C_{14}H_{16}N_2O_4$
2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-
RN: 106231-69-0 **MP** (°C)**:**
MW: 276.29 **BP** (°C)**:** 570.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	B427	1 0 0 1 1	

3296. $C_{14}H_{16}N_2O_4S_2$
4-Thiazolidinecarboxylic acid, 2,2′-(1,4-phenylene)*bis*-
4-Thiazolidinecarboxylic acid, 2,2′-*p*-phenylenebis-
RN: 83690-84-0 **MP** (°C)**:**
MW: 340.42 **BP** (°C)**:** 697.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	6.128E-01	21	B414	1 0 0 1 1	fast decomposition

3297. $C_{14}H_{16}N_4$
Disperse black 3
N,N-Dimethyl-4,4′-azodian
4-Amino-4′-(dimethylamino)azobenzene
C.I. 11025
RN: 539-17-3 **MP** (°C)**:**
MW: 240.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	1.202E-04	25	B333	0 0 0 0 0	

3298. $C_{14}H_{16}N_4O_2S$
2-Sulfanilamido-5,6,7,8-tetrahydroquinazoline
2-Sulfanilamido-5,6,7,8,-tetrahydroquinazoline
RN: 71119-34-1 **MP** (°C)**:** 255
MW: 304.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-04	6.800E-02	29	C049	0 0 0 0 0	

3299. $C_{14}H_{16}N_4O_3S$
*N*4-Acetylsulfamethazine
*N*4-Acetylsulfamezathine
*N*4-Acetylsulphamethazine
Acetylsulfamethazine
2-*p*-Acetamidobenzenesulphonamido-4:6-dimethylpyri-
RN: 100-90-3 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-03	9.291E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
3.590E-03	1.150E+00	37	L091	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	M057	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	R075	1 2 0 0 2	
2.197E-03	7.040E-01	37	S192	1 0 1 1 2	pH 6.0
2.622E-03	8.400E-01	38	K006	1 0 0 0 1	

3300. $C_{14}H_{16}N_4O_3S$
*N*4-Acetylsulphasomidine
Acetamide, *N*-[4-[[(2,6-dimethyl-4-pyrimidinyl)amino]sulfonyl]phenyl]-
RN: 3163-31-3 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.373E-04	4.400E-02	ns	B133	0 2 0 0 1	pH 7.4

3301. $C_{14}H_{16}N_4O_3S$
2-(*N*4-Acetylsulfanilylamino)-4-ethylpyrimidine
RN: **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.435E-05	7.800E-03	37	R076	1 2 0 0 2	

3302. $C_{14}H_{16}N_4O_4S$
*N*4-Acetylsulphamethomidine
RN: **MP** (°C)**:**
MW: 336.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.730E-04	2.600E-01	ns	B133	0 2 0 0 2	pH 7.4

3303. $C_{14}H_{16}N_4O_5S$

*N*4-Acetylsulphadimethoxine
*N*4-Acetyl-2,4-dimethoxy-6-sulfanilamidopyrimidine
*N*4-Acetylsulfadimethoxypyrimidine
Sulfadimethoxine *N*4-acetate
RN: 555-25-9 **MP** (°C)**:**
MW: 352.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.392E-04	1.900E-01	ns	B133	0 2 0 0 2	pH 7.4

3304. $C_{14}H_{16}O_6$

Benzoic acid, 2-(acetyloxy)-, (1-oxobutoxy)methyl ester
RN: 118247-07-7 **MP** (°C)**:** 0il
MW: 280.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.249E-03	3.500E-01	21	N335	0 0 0 0 0	

3305. $C_{14}H_{16}O_6$

Ethylphthalyl ethyl glycolate
Ethoxycarbonylmethyl ethyl phthalate
Ethylphthalyl ethylglycolate
RN: 84-72-0 **MP** (°C)**:** 20
MW: 280.28 **BP** (°C)**:** 320

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-03	<7.99E-01	20	F070	1 0 0 0 1	

3306. $C_{14}H_{17}ClNO_4PS_2$

Dialifos
Dialifor
Diethyl *S*-(2-chloro-1-phthalimidoethyl) phosphorodithioate
Torak
Hercules 14503
RN: 10311-84-9 **MP** (°C)**:** 67
MW: 393.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.570E-07	1.800E-04	ns	F071	0 1 2 1 1	
4.571E-07	1.800E-04	ns	R427	0 0 0 0 0	

3307. $C_{14}H_{17}NO$
1-Cinnamoylpiperidine
N,N-Pentamethylenecinnamamide
1-(1-Oxo-3-phenyl-2-propenyl)-piperidine
RN: 5422-81-1 **MP** (°C)**:**
MW: 215.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	2.067E-01	ns	H350	0 0 0 0 0	

3308. $C_{14}H_{17}NO$
N-Cyclopentylcinnamamide
2-Propenamide, *N*-cyclopentyl-3-phenyl-
RN: 59831-97-9 **MP** (°C)**:**
MW: 215.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.280E-04	4.909E-02	ns	H350	0 0 0 0 0	

3309. $C_{14}H_{17}NO_2S$
m-Carboxylhexylphenylisothiocyanate
3-Carboxylhexylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 263.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.844E-02	25	K032	2 2 0 1 1	

3310. $C_{14}H_{17}NO_3$
Piperidine, 1-[(benzoyloxy)acetyl]-
RN: 106231-67-8 **MP** (°C)**:** 88
MW: 247.30 **BP** (°C)**:** 433.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.154E-03	7.800E-01	22	B427	1 0 0 1 1	
3.154E-03	7.800E-01	22	N317	1 1 2 1 2	

3311. $C_{14}H_{17}NO_4$
4-Piperidinol, 1-[(benzoyloxy)acetyl]-
RN: 115178-71-7 **MP** (°C)**:** 121.5
MW: 263.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.482E-02	1.180E+01	22	N317	1 1 2 1 2	

3312. $C_{14}H_{17}NO_5$

Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-, ethyl ester

RN: 106231-63-4 **MP** (°C)**:** 39.5
MW: 279.30 **BP** (°C)**:** 426.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-02	6.000E+00	22	B427	1 0 0 1 1	in 0.01M HCl
2.148E-02	6.000E+00	22	N317	1 1 2 1 2	

3313. $C_{14}H_{17}N_5O_3$

Pipemidic acid
Pipemidique acide

RN: 51940-44-4 **MP** (°C)**:** 253
MW: 303.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-03	3.215E-01	25	D051	2 0 0 1 2	0.05N NaCl
1.160E-03	3.519E-01	37	D051	2 0 0 1 2	0.05N NaCl

3314. $C_{14}H_{18}ClN_3S$

Chlorothen
N,N-Dimethyl-*N′*-(2-pyridyl)-*N′*-(5-chloro-2-thenyl)ethylenediamine
Chloromethapyrilene
5-Chloro-*N*-(2-(dimethylamino)ethyl)-*N*-(2-pyridyl)-2-thenylamine
Chloropyrilene

RN: 148-65-2 **MP** (°C)**:**
MW: 295.84 **BP** (°C)**:** 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	2.012E+00	37.5	L034	2 2 0 1 2	pH 7.4

3315. $C_{14}H_{18}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *n*-hexyl ester
Chloroxone
Agrotect
Amoxone
BH 2,4-D

RN: 1917-95-9 **MP** (°C)**:**
MW: 305.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.941E-05	5.924E-03	ns	M120	0 0 1 1 2	

3316. $C_{14}H_{18}N_2O$

Propyphenazone
Isopropylantipyrine
1,2-Dihydro-1,5-dimethyl-4-(isopropyl)-2-phenyl-pyrazol-3-one
4-Isopropyl-2,3-dimethyl-5-oxo-1-phenyl-3-pyrazoline
RN: 479-92-5 **MP** (°C)**:** 103
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.383E+00	7.791E+02	4.62	M109	2 1 1 1 0	EFG
3.330E+00	7.670E+02	10.93	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	15.02	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	20.96	M109	2 1 1 1 0	EFG
3.229E+00	7.436E+02	25.35	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	29.87	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	38.37	M109	2 1 1 1 0	EFG
3.348E+00	7.711E+02	40.32	M109	2 1 1 1 0	EFG

3317. $C_{14}H_{18}N_2O_3$

Reposal
5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetri-one
5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethylbarbituric acid
RN: 3625-25-0 **MP** (°C)**:** 213
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-03	4.407E-01	25	V033	2 0 1 1 2	
1.700E-03	4.459E-01	25.00	T303	1 0 0 0 1	
2.300E-03	6.033E-01	35.00	T303	1 0 0 0 1	
2.500E-03	6.558E-01	45.00	T303	1 0 0 0 1	

3318. $C_{14}H_{18}N_2O_3$

Piperazine, 1-[(benzoyloxy)acetyl]-4-methyl-
RN: 106231-70-3 **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:** 438.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>7.62E-01	>2.00E+02	22	B427	1 0 0 1 1	

3319. $C_{14}H_{18}N_4O_2S$

2-Sulfanilylamino-4-isobutylpyrimidine
RN: 106596-34-3 **MP** (°C)**:**
MW: 306.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.264E-04	1.000E-01	37	R076	1 2 0 0 1	

3320. $C_{14}H_{18}N_4O_3$

Benomyl
(1-(Butylamino)carbonyl)-1H-benzimidazol-2-yl)carbamic acid methyl ester
RN: 17804-35-2 **MP** (°C)**:**
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	3.800E-03	20	A064	1 0 1 1 1	
1.309E-05	3.800E-03	20	M161	1 0 0 0 1	pH 7
~6.89E-06	~2.00E-03	ns	B309	0 0 0 0 0	

3321. $C_{14}H_{18}N_4O_3$

Trimethoprim
5-(3,4,5-Trimethoxybenzyl)-2,4-diaminopyrimidine
Monotrim
Syraprim
Proloprim
Trimpex
RN: 738-70-5 **MP** (°C)**:** 201
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	1.752E-02	22.5	B440	0 0 0 0 0	
1.396E-03	4.053E-01	25	H434	0 0 0 0 0	
1.378E-03	4.000E-01	25	M167	1 0 0 0 0	
1.722E-03	5.000E-01	32	D308	0 0 0 0 0	pH 8.54
2.711E-03	7.870E-01	37	G086	1 0 0 0 1	
1.378E-03	4.000E-01	37	M321	1 0 0 0 2	intrinsic
>1.72E-03	>5.00E-01	ns	B404	0 2 1 1 0	
1.378E-03	4.000E-01	ns	K444	0 0 0 0 0	

3322. $C_{14}H_{18}N_4O_6.0.5H_2O$

2′-Propionyl-6-methoxypurine arabinoside (hemihydrate)
RN: 145913-38-8 **MP** (°C)**:** 60–65
MW: 347.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-01	3.821E+01	37	C348	0 0 0 0 0	pH 7.00

3323. $C_{14}H_{18}N_4O_7.0.5H_2O$

9-[5-*O*-(Methoxyacetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 121032-38-0 **MP** (°C)**:** 137–139
MW: 363.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-02	2.838E+01	37	M378	1 2 1 1 2	pH 7.2

3324. $C_{14}H_{18}N_4O_7.0.9H_2O$

2′-Methoxyacetyl-6-methoxypurine arabinoside (0.9 hydrate)

RN: 145913-47-9 **MP** (°C)**:**
MW: 370.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.090E-02	3.368E+01	37	C348	0 0 0 0 0	pH 7.00

3325. $C_{14}H_{18}N_6O$

(1S,4R)-4-[2-Amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol sulfate (salt)

ABC sulfate[47]

ABC[48]

Abacavir

RN: 188062-50-2 **MP** (°C)**:**
MW: 286.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.867E-09	1.680E-06	32	M458	0 0 0 0 0	

3326. $C_{14}H_{18}N_6O_4$

2,5-Diaziridinyl-3,6-bis(glycinamide)-1,4-benzoquinone

RN: 59886-49-6 **MP** (°C)**:** 200
MW: 334.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.495E-03	5.000E-01	rt	C317	0 0 0 0 0	

3327. $C_{14}H_{18}O_4$

Diisopropyl phthalate

bis(1-Methyl-ethyl) phthalate

RN: 605-45-8 **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-03	3.329E-01	20	L300	2 1 0 2 2	

3328. $C_{14}H_{18}O_4$
Di-*n*-propyl phthalate
Dipropyl phthalate
RN: 131-16-8 **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-04	1.081E-01	20	L300	2 1 0 2 2	

3329. $C_{14}H_{18}O_4$
Diisopropyl *o*-phthalate
RN: **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-04	1.670E-01	25	S417	0 0 0 0 0	

3330. $C_{14}H_{18}O_6$
Methyl glycol phthalate
bis(2-Methoxyethyl) phthalate
RN: 117-82-8 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-02	8.723E+00	15	H069	1 0 1 1 1	

3331. $C_{14}H_{18}O_6$
Ethyl phthalyl ethyl glycollate
RN: **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-03	4.998E-01	15	H069	1 0 1 1 0	
1.770E-03	4.998E-01	ns	F014	0 0 0 0 1	

3332. $C_{14}H_{18}O_6$
Dimethoxyethyl phthalate
1,2-Benzenedicarboxylic acid, di(2-methoxyethyl) ester
RN: 34006-76-3 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.986E-02	8.428E+00	20	F070	1 0 0 0 1	
2.944E-02	8.310E+00	ns	F014	0 0 0 0 2	

3333. $C_{14}H_{19}Cl_2NO_2$

Chlorambucil
N,N-di-(2-Chloroethyl)-γ-(*p*-aminophenyl)butyric acid
Linfolysin
Elcoril
Linfolizin
Leukersan

RN: 305-03-3 **MP** (°C)**:** 64
MW: 304.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	9.127E-02	3	G434	0 0 0 0 0	pH 4.13
<3.29E-03	<1.00E+00	30	L343	2 1 1 1 0	EFG

3334. $C_{14}H_{19}IN_2O_6$

Uridine, 2′-deoxy-5-iodo-, 5′-pentanoate
5′-Valeryl 5-iodo-2′-deoxyuridine

RN: 84052-69-7 **MP** (°C)**:** 142.5
MW: 438.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E+02	1.753E+05	25	N332	0 0 0 0 0	pH 7.4

3335. $C_{14}H_{19}IN_2O_6$

Uridine, 2′-deoxy-5-iodo-, 5′-(2,2-dimethylpropanoate)
5′-Pivaloyl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-pivalate

RN: 84043-28-7 **MP** (°C)**:** 106.5
MW: 438.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E+02	1.928E+05	25	N332	0 0 0 0 0	pH 7.4

3336. $C_{14}H_{19}NO$

n-Pentylcinnamamide
2-Propenamide, *N*-pentyl-3-phenyl-

RN: 23784-51-2 **MP** (°C)**:**
MW: 217.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.782E-02	ns	H350	0 0 0 0 0	

3337. $C_{14}H_{19}NO_3$
Acetaminophen hexanoate
Hexanyl acetaminophen
Hexanoic acid, 4-(acetylamino)phenyl ester
4′-Hydroxyacetanilide hexanoate
RN: 20675-21-2 **MP** (°C)**:** 107
MW: 249.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.220E-05	1.800E-02	25	B010	1 1 1 1 0	
2.286E-04	5.700E-02	37	D029	0 0 0 0 0	

3338. $C_{14}H_{19}NO_3$
Propanamide, 2-(benzoyloxy)-*N*,*N*-diethyl-
RN: 115178-79-5 **MP** (°C)**:** 53.5
MW: 249.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.214E-03	1.300E+00	22	N317	1 1 2 1 2	

3339. $C_{14}H_{19}NO_4$
Anisomycin
(2R,3R,4R)-2-(4-Methoxybenzyl)-3,4-pyrrolidinediol-3-acetate
RN: 22862-76-6 **MP** (°C)**:** 140.5
MW: 265.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	6.550E+00	28	A038	2 0 1 1 2	

3340. $C_{14}H_{19}N_3S$
Methapyrilene
N,*N*-Dimethyl-*N*′,2-pyridinyl-*N*′-(2-thienylmethyl)-1,2-ethanediamine
Cope
A 3322
AH-42
Semiken
RN: 91-80-5 **MP** (°C)**:** <25
MW: 261.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	6.012E-01	30	L068	1 0 0 1 0	EFG
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3341. $C_{14}H_{19}N_3S$

Thenyldiamine
1,2-Ethanediamine, *N,N*-dimethyl-*N′*-2-pyridinyl-*N′*-(3-thienylmethyl)-
N-(2-Dimethylaminoethyl)-*N*-2-pyridyl-3-thenylamine
Thefanil
Thenfadil
Tenfidil

RN: 91-79-2 **MP** (°C)**:**
MW: 261.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3342. $C_{14}H_{19}N_5O_4$

N,N-Diethylsuccinamyloxymethyl-1-allopurinol
Butanoic acid, 4-(diethylamino)-4-oxo-, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl) methyl ester

RN: 98827-27-1 **MP** (°C)**:** 138-140
MW: 321.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.027E-01	3.300E+01	22	B322	0 0 0 0 0	

3343. $C_{14}H_{19}N_5O_5$

9-[5′-(*O*-Butyryl)-β-D-arabinofuranosyl]adenine ester
Vidarabine 5′-butyrate

RN: 65926-30-9 **MP** (°C)**:**
MW: 337.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-02	1.610E+01	ns	B134	0 1 1 1 2	

3344. $C_{14}H_{19}O_6P$

Crotoxyphos
Dimethylphosphate of α-methylbenzyl-3-hydroxy-*cis*-crotonate

RN: 7700-17-6 **MP** (°C)**:**
MW: 314.28 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.179E-03	9.990E-01	ns	M061	0 0 0 0 0	
3.182E-03	1.000E+00	rt	M161	0 0 0 0 0	

3345. $C_{14}H_{20}ClNO_2$

Alachlor
2-Chloro-2′,6′-diethyl-*N*-(methoxymethyl)acetanilide
RN: 15972-60-8 **MP** (°C)**:** 39.5
MW: 269.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-04	2.400E-01	23	M161	1 0 0 0 2	
5.486E-04	1.480E-01	25	B200	1 0 0 0 2	
5.486E-04	1.480E-01	ns	M061	0 0 0 0 2	
5.560E-04	1.500E-01	ns	M110	0 0 0 0 0	EFG
8.896E-04	2.400E-01	ns	V414	0 0 0 0 0	

3346. $C_{14}H_{20}ClNO_2$

Acetochlor
Doubleplay
Harness
Topnotch
Top Hand
Acenit
RN: 34256-82-1 **MP** (°C)**:**
MW: 269.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.260E-04	2.228E-01	ns	S460	0 0 0 0 0	

3347. $C_{14}H_{20}N_2O$

Siduron
1-(2-Methylcyclohexyl)-3-phenylurea
RN: 1982-49-6 **MP** (°C)**:** 133
MW: 232.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.748E-05	1.800E-02	25	B200	1 0 0 0 1	
7.748E-05	1.800E-02	25	G036	1 0 0 0 1	
7.748E-05	1.800E-02	25	M161	1 0 0 0 1	

3348. $C_{14}H_{20}N_2O_2$
Pindolol
Barbloc
Visken
2-Propanol, 1-(1H-indol-4-yloxy)-3-[(-methylethyl)amino]-
RN: 13523-86-9 **MP** (°C)**:**
MW: 248.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-04	3.300E-02	22.5	B422	2 0 2 2 2	

3349. $C_{14}H_{20}N_2O_3S$
Tolcyclamide
1-Cyclohexyl-3-*para*-tolylsulfonylurea
Glycyclamide
RN: 664-95-9 **MP** (°C)**:** 175
MW: 296.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.194E-05	1.836E-02	37	A028	1 0 2 1 2	intrinsic
6.200E-05	1.838E-02	37	A046	2 0 1 1 2	

3350. $C_{14}H_{20}N_3O_5PS$
Pyrazophos
2-[(Diethoxyphosphinothioyl)oxy]-5-methylpyrazolo[1,5-a]pyrimidine-6-carboxylic acid ethyl Ester
Afugan
Curamil
RN: 13457-18-6 **MP** (°C)**:** 50.5
MW: 373.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.125E-05	4.200E-03	20	A306	0 0 0 0 0	
1.125E-05	4.200E-03	20	M161	1 0 0 0 1	

3351. $C_{14}H_{20}N_4O_2$
2,5-bis(Methylaziridinyl)-3,6-bis(methylamino)-1,4-benzoquinone
RN: 64947-06-4 **MP** (°C)**:** 179
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.62E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3352. $C_{14}H_{20}N_4O_2$

2,5-Diaziridinyl-3,6-bis(dimethylamino)-1,4-benzoquinone

RN: 59886-50-9 **MP** (°C)**:** 112
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-02	1.000E+01	rt	C317	0 0 0 0 0	

3353. $C_{14}H_{20}N_4O_2$

2,5-Diaziridinyl-3,6-bis(ethylamino)-1,4-benzoquinone

RN: 59886-53-2 **MP** (°C)**:** 157
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.809E-03	5.000E-01	rt	C317	0 0 0 0 0	

3354. $C_{14}H_{20}N_4O_4$

2,5-Diaziridinyl-3,6-bis(hydroxyethylamino)-1,4-benzoquinone

RN: 59886-54-3 **MP** (°C)**:** 188
MW: 308.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-03	2.000E+00	rt	C317	0 0 0 0 0	

3355. $C_{14}H_{20}O_3$

Heptyl *p*-hydroxybenzoate
n-Heptyl 4-hydroxybenzoate

RN: 1085-12-7 **MP** (°C)**:** 48
MW: 236.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	6.215E-02	–244	B355	0 0 0 0 0	
2.010E-04	4.750E-02	15	B355	0 0 0 0 0	
2.520E-04	5.955E-02	20	B355	0 0 0 0 0	
5.827E-03	1.377E+00	25	D081	1 2 2 1 2	*sic*
1.259E-04	2.975E-02	25	F322	2 0 1 1 0	EFG

3356. $C_{14}H_{21}NO_2$
Heptyl *p*-aminobenzoate
Heptyl 4-aminobenzoate
RN: 14309-40-1 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	4.707E-03	37	F006	1 1 2 2 1	
3.300E-05	7.766E-03	ns	M066	0 0 0 0 1	

3357. $C_{14}H_{21}NO_2$
2,6-Diisopropyl-4-acetaminophenol
3,5-Diisopropylparacetamol
4-Acetamido-2,6-diisopropylphenol
RN: 1988-14-3 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.844E-04	1.375E-01	25	D078	1 2 2 1 2	

3358. $C_{14}H_{21}NO_2$
Octyl nicotinate
Nicotinic acid *n*-octyl ester
RN: 70136-02-6 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.249E-05	1.000E-02	32	L346	1 0 0 1 2	

3359. $C_{14}H_{21}NO_2$
Benzeneacetamide, *N*-hydroxy-α-dipropyl
RN: 60631-09-6 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	3.059E-01	26	G076	1 0 0 0 1	

3360. $C_{14}H_{21}NO_2$
Benzenepropanamide, *N*-hydroxy-α2,4,6-pentamethyl
RN: 60631-10-9 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.060E-02	26	G076	1 0 0 0 1	

3361. $C_{14}H_{21}NO_3$

4-Methoxybenzoic acid-2-(diethylamino)ethyl ester
Diethylaminoethyl *p*-anisate
RN: 10367-84-7 **MP** (°C)**:**
MW: 251.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.332E+00	ns	M066	0 0 0 0 1	

3362. $C_{14}H_{21}NO_4P$

Phenyl(di-morpholido)-phosphate
RN: **MP** (°C)**:**
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	7.706E+02	25	A040	1 0 0 0 2	

3363. $C_{14}H_{21}N_3O_3$

Karbutilate
m-(3,3-Dimethylureido)phenyl-*tert*-butylcarbamate
Tandex
RN: 4849-32-5 **MP** (°C)**:** 176.3
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-03	3.250E-01	20	B200	1 0 0 0 2	
1.163E-03	3.250E-01	rt	M161	0 0 0 0 2	

3364. $C_{14}H_{21}N_3O_3S$

Tolazamide
N-(((Hexahydro-1H-azepin-1-yl)amino)carbonyl)-4-methylbenzenesulfonamide
Tolinase
N-(*p*-Toluenesulfonyl)-*N′*-hexamethyleniminourea
U 17835
RN: 1156-19-0 **MP** (°C)**:** 170
MW: 311.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.540E-02	30	H025	1 0 2 1 1	intrinsic
1.124E-03	3.499E-01	ns	B404	0 2 1 1 0	

3365. $C_{14}H_{22}$

2-Octylbenzene
(1-Methylheptyl)benzene
RN: 777-22-0 **MP** (°C)**:**
MW: 190.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-06	3.017E-04	ns	D001	0 0 0 0 2	

3366. $C_{14}H_{22}N_2O$

Lidocaine
2-(Diethylamino)-*N*-(2,6-dimethylphenyl)acetamide
2-Diethylamino-2′,6′-acetoxylidide
Lignocaine
Leostesin
Xylocaine
RN: 137-58-6 **MP** (°C)**:** 68
MW: 234.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-02	4.335E+00	14.5	N046	2 0 1 1 1	intrinsic
5.460E-05	1.279E-02	22.5	B440	0 0 0 0 0	
1.550E-02	3.632E+00	25	D402	1 2 2 2 0	EFG
1.643E-02	3.850E+00	25	L338	1 0 1 1 2	
1.630E-02	3.820E+00	25	N046	2 0 1 1 1	intrinsic
1.488E-02	3.488E+00	25	S450	0 0 0 0 0	Intrinsic
1.750E-02	4.101E+00	30	L068	1 0 0 1 0	EFG
1.460E-02	3.421E+00	34.5	N046	2 0 1 1 1	intrinsic
1.700E-02	3.984E+00	37	D402	1 2 2 2 0	
1.440E-02	3.375E+00	37	N044	2 1 1 2 2	intrinsic

3367. $C_{14}H_{22}N_2O_2$

4-Methylaminobenzoic acid-2-(diethyl-amino)ethyl ester
Benzoic acid, 4-(methylamino)-, 2-(diethylamino)ethyl ester
Benzoic acid, *p*-(methylamino)-, 2-(diethylamino)ethyl ester
RN: 16488-52-1 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-03	1.940E+00	ns	M066	0 0 0 0 2	

3368. $C_{14}H_{22}N_2O_2$
4-Aminobenzoic acid-2-(diethyl-amino)propyl ester
2-Diethylamino)propyl 4-aminobenzoate
RN: 5878-13-7 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.229E+00	ns	M066	0 0 0 0 2	

3369. $C_{14}H_{22}N_2O_3$
2,4-Diazaspiro[5.10]hexadecane-1,3,5-trione
RN: 143288-63-5 **MP** (°C)**:**
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	6.925E-03	25	P350	0 0 0 0 0	intrinsic

3370. $C_{14}H_{22}N_2O_3$
Atenolol
Anselol
Apo-atenolol
Benzeneacetamide
4-(2′-Hydroxy-3′-((1-methylethyl)amino)propoxy)-
Noten
RN: 29122-68-7 **MP** (°C)**:**
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.069E-05	1.350E-02	25	A408	2 0 1 2 0	int
7.134E-10	1.900E-07	32	M458	0 0 0 0 0	
9.950E-02	2.650E+01	ns	K444	0 0 0 0 0	

3371. $C_{14}H_{22}N_2O_4$
Ethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate
Ethyl 2-methyl-2-cyclohexenyl-6-methylmalonurate
RN: **MP** (°C)**:** 97.5
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.823E-01	23	B152	1 2 1 1 1	pH 3.5

3372. $C_{14}H_{22}N_2O_5$

Methoxymethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate

RN: **MP** (°C)**:** 73
MW: 298.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	1.134E+00	23	B152	1 2 1 1 1	pH 3.5

3373. $C_{14}H_{22}O$

Methyl ionone
6-Methylionone

RN: 1335-46-2 **MP** (°C)**:**
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.693E-05	2.000E-02	25	M350	1 0 1 1 1	

3374. $C_{14}H_{22}O$

o-*n*-Octylphenol
2-*n*-Octylphenol

RN: 949-13-3 **MP** (°C)**:**
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	2.857E-03	25	L022	1 0 0 0 0	

3375. $C_{14}H_{22}O$

p-*n*-Octylphenol
4-Octylphenol

RN: 1806-26-4 **MP** (°C)**:** 44.5
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.107E-05	1.260E-02	20.5	A335	0 0 0 0 0	
6.120E-05	1.263E-02	20.5	A335	0 0 0 0 0	
8.812E-06	1.818E-03	25	L022	1 0 0 0 0	

3376. $C_{14}H_{23}O_3P$

Dibutyl phenyl phosphonate
Dibutoxyphenylphosphine oxide
Dibutyl phenylphosphonate
RN: 1024-34-6 **MP** (°C)**:**
MW: 270.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.40E-04	<2.00E-01	25	B070	1 2 0 1 0	

3377. $C_{14}H_{24}NO_4PS_3$

Bensulide
O,O-bis(1-Methylethyl) *S*-(2-((phenylsulfonyl)amino)ethyl) phosphorodithioate
Betasan
Betamec
Exporsan
Benzulfide
RN: 741-58-2 **MP** (°C)**:** 34.4
MW: 397.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-05	2.500E-02	20	B200	1 2 0 0 1	
6.289E-05	2.500E-02	rt	M161	0 0 0 0 1	

3378. $C_{14}H_{24}N_2O_3$

5-Ethyl-5-*n*-octylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-octyl-
5-Ethyl-5-octylbarbiturate
RN: 64810-90-8 **MP** (°C)**:**
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	3.059E-02	25	M310	2 2 2 2 2	

3379. $C_{14}H_{24}N_2O_3$

p-5-Ethyl-5-methylhexylcarbinylbarbituric acid
RN: **MP** (°C)**:**
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-03	4.140E-01	ns	T003	0 0 0 0 2	

3380. $C_{14}H_{24}O_2$

3-Hydroxy-2,5-dispirocyclohexyltetrahydrofuran
7-Oxadispiro[5.1.5.2]pentadecan-14-ol
RN: 29839-63-2 **MP** (°C)**:**
MW: 224.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.098E-02	6.951E+00	rt	B066	0 2 0 0 0	contains impurity

3381. $C_{14}H_{26}O_4$

1,12-Dodecanedicarboxylic acid
Tetradecanedioic acid
RN: 821-38-5 **MP** (°C)**:** 127
MW: 258.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.741E-04	2.000E-01	21	B040	1 0 1 1 0	*sic*

3382. $C_{14}H_{27}NO_2$

Pentanamide,*N*-hydroxy-α,α-dipropyl
RN: **MP** (°C)**:**
MW: 241.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.207E-01	26	G076	1 0 0 0 1	

3383. $C_{14}H_{28}NO_3PS_2$

Piperophos
S-(2-(2-Methyl-1-piperidinyl)-2-oxoethyl) *O,O*-dipropyl phosphorodithioate
RN: 24151-93-7 **MP** (°C)**:**
MW: 353.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.072E-05	2.500E-02	20	M161	1 0 0 0 1	

3384. $C_{14}H_{28}N_2O_2$

N,N,N′,N′-Tetramethylsebacamide
Decanediamide, *N,N,N′,N′*-tetramethyl-
RN: 13424-83-4 **MP** (°C)**:**
MW: 256.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.270E-01	1.351E+02	30	D010	1 2 1 1 2	

3385. $C_{14}H_{28}O_2$

Myristic acid
Tetradecanoic acid
Crodacid
1-Tridecanecarboxylic acid

RN: 544-63-8 **MP** (°C)**:** 54
MW: 228.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.692E-05	1.300E-02	0	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	D041	1 0 0 0 0	
8.757E-05	2.000E-02	20	R001	1 1 1 1 1	
4.700E-06	1.073E-03	25	J001	1 0 2 1 1	average of 2
8.000E-07	1.827E-04	25	R002	0 0 0 0 0	intrinsic
3.710E-06	8.473E-04	25	R002	0 0 0 0 0	
9.633E-05	2.200E-02	30	B136	1 0 2 1 1	
1.051E-04	2.400E-02	30	R001	1 1 1 1 1	
1.270E-04	2.900E-02	40	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	R001	1 1 1 1 1	
1.839E-05	4.200E-03	50	E005	2 1 1 2 1	
9.700E-06	2.215E-03	50	J001	1 0 2 1 1	
1.489E-04	3.400E-02	60	B136	1 0 2 1 1	
2.452E-05	5.600E-03	60	E005	2 1 1 2 1	
1.489E-04	3.400E-02	60	R001	1 1 1 1 1	
5.692E-05	1.300E-02	.0	R001	1 1 1 1 1	

3386. $C_{14}H_{28}O_4$

1,3-Dioxolane-4-methanol, 2-[2-(heptyloxy)ethyl]-2-methyl

RN: 143458-57-5 **MP** (°C)**:**
MW: 260.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.440E-03	1.156E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

3387. $C_{14}H_{29}NO_2$

Benzenepropanamide, *N*-hydroxy-α2,3-pentamethyl
Octanamide, *N*-hydroxy-2,2-dipropyl

RN: 60631-08-5 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	
1.500E-03	3.651E-01	26	G076	1 0 0 0 1	

3388. $C_{14}H_{29}NO_2$
Octanamide, 2,2,4-triethyl-*N*-hydroxy
RN: 60631-07-4 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	

3389. $C_{14}H_{29}NO_2$
Decanamide, 2,2-diethyl-*N*-hydroxy
RN: 60631-06-3 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.460E-03	26	G076	1 0 0 0 1	

3390. $C_{14}H_{29}NO_2$
Dodecanamide, *N*-hydroxy-2,2-dimethyl
RN: 60631-05-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.894E-03	26	G076	1 0 0 0 1	

3391. $C_{14}H_{29}NO_2$
Pentanamide, *N*-hydroxy-4-methyl-2,2-bis(2-methylpropyl)
RN: 60469-53-6 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+01	2.434E+03	26	G076	1 0 0 0 1	

3392. $C_{14}H_{29}NO_2$
Hexanamide, 2,2-dibutyl-*N*-hydroxy
2,2-Dibutyl-*N*-hydroxyhexanamide
Tri-*n*-butylacetohydroxamic acid
RN: 52061-82-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.704E-02	26	G076	1 0 0 0 1	

3393. $C_{14}H_{29}NO_2$

Tetradecanamide, *N*-hydroxy
Myristohydroxamic acid
N-Hydroxytetradecanamide
RN: 17698-03-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-04	2.434E-02	26	G076	1 0 0 0 1	

3394. $C_{14}H_{30}$

n-Tetradecane
Tetradecane
RN: 629-59-4 **MP** (°C)**:** 5.89
MW: 198.40 **BP** (°C)**:** 253.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.663E-09	3.300E-07	23	C332	0 0 0 0 0	
3.500E-08	6.944E-06	25	F004	0 0 0 0 0	
1.159E-08	2.300E-06	ns	H123	0 0 0 0 0	

3395. $C_{14}H_{30}O$

Tetradecanol
RN: 27196-00-5 **MP** (°C)**:**
MW: 214.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-06	3.130E-04	25	R002	0 0 0 0 0	

3396. $C_{14}H_{30}O$

Myristyl alcohol
Tetradecanol
RN: 112-72-1 **MP** (°C)**:** 38
MW: 214.39 **BP** (°C)**:** 289

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.049E-08	1.940E-05	4	H030	2 2 2 2 2	
9.049E-08	1.940E-05	4	H103	1 2 2 2 2	
8.909E-07	1.910E-04	25	H103	1 2 2 2 2	
5.737E-07	1.230E-04	32	H030	2 2 2 2 2	
5.737E-07	1.230E-04	32	H103	1 2 2 2 2	
1.105E-06	2.370E-04	45	H030	2 2 2 2 2	
1.105E-06	2.370E-04	45	H103	1 2 2 2 2	
2.094E-06	4.490E-04	61	H030	2 2 2 2 2	
2.094E-06	4.490E-04	61	H103	1 2 2 2 2	

3397. $C_{14}H_{31}O_2P$

Ethyl dihexyl phosphinate
Phosphinic acid, dihexyl-, ethyl ester
RN: 113977-19-8 **MP** (°C)**:**
MW: 262.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.81E-04	<1.00E-01	25	B070	1 2 0 1 0	

3398. $C_{14}H_{31}O_3P$

Dibutyl hexyl phosphonate
Phosphinic acid, hexyl-, dibutyl ester
RN: 5929-66-8 **MP** (°C)**:**
MW: 278.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.18E-04	<2.00E-01	25	B070	1 2 0 1 0	

3399. $C_{14}H_{31}O_3P$

Diethyl hexyl phosphonate
Phosphinic acid, hexyl-, diethyl ester
RN: 16165-66-5 **MP** (°C)**:**
MW: 278.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.155E-03	6.000E-01	25	B070	1 2 0 1 0	

3400. $C_{14}H_{31}O_4P$

Dibutyl hexyl phosphate
Phosphoric acid, dibutyl hexyl ester
RN: 80421-90-5 **MP** (°C)**:**
MW: 294.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3401. $C_{14}H_{31}O_4P$

Diethyl decyl phosphate
Phosphoric acid, decyl ester
RN: 20195-16-8 **MP** (°C)**:**
MW: 294.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3402. $C_{14}H_{31}O_5P$
Dibutyl ethoxybutyl phosphate
RN: 100888-67-3 **MP** (°C)**:**
MW: 310.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	7.000E-01	25	B070	1 2 0 1 0	

3403. $C_{15}H_{10}$
4,5-Methylenephenanthrene
4H-Cyclopenta[def]phenanthrene
RN: 203-64-5 **MP** (°C)**:** 76
MW: 190.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.782E-06	1.100E-03	27	D003	1 0 0 1 1	

3404. $C_{15}H_{10}Cl_2N_2O_2$
Lorazepam
Alzapam
Ativan
Apo-lorazepam
7-Chloro-5-(*o*-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
RN: 846-49-1 **MP** (°C)**:** 167
MW: 321.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.681E-04	5.400E-02	ns	N315	0 2 2 1 2	pH 7.09

3405. $C_{15}H_{10}O_2$
9-Anthracenecarboxylic acid
Anthracene-9-carboxylic acid
RN: 723-62-6 **MP** (°C)**:** 214
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.824E-04	8.499E-02	24	H106	1 0 2 2 2	
3.825E-07	8.500E-05	ns	M349	0 2 1 1 2	

3406. $C_{15}H_{10}O_4S$
7-Methylthio-2-xanthonecarboxylic acid
RN: 40363-76-6 **MP** (°C)**:**
MW: 286.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.081E-07	2.600E-04	25	C059	1 2 1 1 1	

3407. $C_{15}H_{10}O_5S$
7-Methylsulfinyl-2-xanthonecarboxylic acid
RN: 40691-50-7 **MP** (°C)**:**
MW: 302.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.064E-06	2.740E-03	25	C059	1 2 1 1 2	

3408. $C_{15}H_{10}O_6$
Eriodictyol
5,7,3′,4′-Tetra-hydroxyflavon
RN: 552-58-9 **MP** (°C)**:** 257dec
MW: 286.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.445E-04	7.000E-02	20	F300	1 0 0 0 1	
6.987E-04	2.000E-01	100	F300	1 0 0 0 2	

3409. $C_{15}H_{10}O_7$
Morin
3,5,7,2′,4′,-Penta-hydroxyflavon
RN: 480-16-0 **MP** (°C)**:** 299.5
MW: 302.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.271E-04	2.500E-01	20	F300	1 0 0 0 1	
2.978E-03	9.000E-01	100	F300	1 0 0 0 0	

3410. $C_{15}H_{10}O_7$

Quarcetin
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one
3,3′,4′,5,7-Pentahydroxyflavone
3′,4′,5,7-Tetrahydroxyflavon-3-ol
Xanthaurine
Meletin

RN: 117-39-5 **MP** (°C)**:** 316–317
MW: 302.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.985E-02	6.000E+00	ns	Z411	0 0 0 0 0	

3411. $C_{15}H_{10}O_7.H_2O$

Morin hydrate
4H-1-Benzopyran-4-one, 2-(2,4-dihydroxyphenyl)-3,5,7-trihydroxy-, monohydrate
Flavone, 2′,3,4′,5,7-pentahydroxy-, monohydrate
Morin monohydrate

RN: 6202-27-3 **MP** (°C)**:**
MW: 320.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-04	1.920E-01	ns	B404	0 2 1 1 0	

3412. $C_{15}H_{11}ClF_3NO_4$

Oxyfluorfen
Oxyfluorofen
Koltar
Goal
2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene
Goal 1.6E

RN: 42874-03-3 **MP** (°C)**:** 83–84
MW: 361.71 **BP** (°C)**:** >240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.236E-07	1.170E-04	ns	R427	0 0 0 0 0	

3413. $C_{15}H_{11}ClN_2O_2$

Oxazepam
Serax
7-Chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one
Apo-oxazepam
Abboxampam

RN: 604-75-1 **MP** (°C)**:** 205.5
MW: 286.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-05	2.000E-02	22	N319	0 0 0 0 0	
1.744E-04	5.000E-02	amb	L434	0 0 0 0 0	
7.673E-05	2.200E-02	c	B362	0 0 0 0 0	

3414. $C_{15}H_{11}ClO_3$

Chlorflurecol-methyl
Chlorflurenol
Methyl-2-chloro-9-hydroxyfluorene-9-carboxylate

RN: 2536-31-4 **MP** (°C)**:** 152
MW: 274.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.552E-05	1.800E-02	20	A308	1 0 0 0 1	
7.936E-05	2.180E-02	20	B200	1 0 0 0 2	
6.552E-05	1.800E-02	20	M161	1 0 0 0 1	

3415. $C_{15}H_{11}NO_2$

C.I. Disperse orange 11
1-Amino-2-methylanthraquinone
2-Methyl-1-anthraquinonylamine
Acetate fast orange R

RN: 82-28-0 **MP** (°C)**:** 208
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.322E-04	25	B333	0 0 0 0 0	

3416. $C_{15}H_{11}NO_2$

C.I. Disperse red 9
1-(Methylamino)-9,10-anthraquinone
Serilene fast pink BT
Smoke red M

RN: 82-38-2 **MP** (°C)**:** 161
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-07	7.355E-05	25	B333	0 0 0 0 0	

3417. $C_{15}H_{11}NO_3$

N-epoxymethyl-1,8-naphthamilide
ENA

RN: **MP** (°C)**:**
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.580E-05	1.160E-02	ns	D428	0 0 0 0 0	

3418. $C_{15}H_{11}N_3$

2,2′,6,2″-terpyridine
Terpyridine
Tripyridyl

RN: 1148-79-4 **MP** (°C)**:**
MW: 233.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.310E-03	1.472E+00	24.99	B444	0 0 0 0 0	

3419. $C_{15}H_{11}N_3O_3$

Nitrazepam
1,3-Dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one
Mogadon
Unisomnia

RN: 146-22-5 **MP** (°C)**:** 224
MW: 281.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	4.300E-02	30	O321	0 0 0 0 0	

3420. $C_{15}H_{12}$

1-Methylphenanthrene

RN: 832-69-9 **MP** (°C)**:** 118
MW: 192.26 **BP** (°C)**:** 358

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-07	9.520E-05	6.60	M063	2 1 2 2 2	
4.950E-07	9.517E-05	6.60	M082	1 1 1 2 2	
4.950E-07	9.517E-05	6.60	M151	2 1 2 2 2	
4.956E-06	9.529E-04	6.64	M183	1 2 1 1 2	
5.929E-07	1.140E-04	8.90	M063	2 1 2 2 2	
5.940E-07	1.142E-04	8.90	M082	1 1 1 2 2	
5.940E-07	1.142E-04	8.90	M151	2 1 2 2 2	
5.933E-07	1.141E-04	8.94	M183	1 2 1 1 2	
7.646E-07	1.470E-04	14.00	M063	2 1 2 2 2	
7.650E-07	1.471E-04	14.00	M082	1 1 1 2 2	
7.650E-07	1.471E-04	14.00	M151	2 1 2 2 2	
7.650E-07	1.471E-04	14.04	M183	1 2 1 1 2	
1.004E-06	1.930E-04	19.20	M063	2 1 2 2 2	
1.010E-06	1.942E-04	19.20	M082	1 1 1 2 2	
1.010E-06	1.942E-04	19.20	M151	2 1 2 2 2	
1.004E-06	1.931E-04	19.24	M183	1 2 1 1 2	
1.326E-06	2.550E-04	24.10	M063	2 1 2 2 2	
1.320E-06	2.538E-04	24.10	M082	1 1 1 2 2	
1.320E-06	2.538E-04	24.10	M151	2 1 2 2 2	
1.327E-06	2.552E-04	24.14	M183	1 2 1 1 2	
1.399E-06	2.690E-04	25.00	M151	2 1 1 2 2	
1.581E-06	3.040E-04	26.90	M063	2 1 2 2 2	
1.580E-06	3.038E-04	26.90	M082	1 1 1 2 2	
1.580E-06	3.038E-04	26.90	M151	2 1 2 2 2	
1.583E-06	3.043E-04	26.94	M183	1 2 1 1 2	
1.846E-06	3.550E-04	29.90	M063	2 1 2 2 2	
1.850E-06	3.557E-04	29.90	M082	1 1 1 2 2	
1.850E-06	3.557E-04	29.90	M151	2 1 2 2 2	
1.848E-06	3.553E-04	29.94	M183	1 2 1 1 2	

3421. $C_{15}H_{12}$

2-Methylanthracene

RN: 613-12-7 **MP** (°C)**:** 204
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-08	7.060E-06	6.30	M063	2 1 2 2 2	
3.670E-08	7.056E-06	6.30	M082	1 1 1 2 2	
3.670E-08	7.056E-06	6.30	M151	2 1 2 2 2	
3.675E-08	7.066E-06	6.34	M183	1 2 1 1 2	
4.411E-08	8.480E-06	9.10	M063	2 1 2 2 2	
4.410E-08	8.479E-06	9.10	M082	1 1 1 2 2	
4.410E-08	8.479E-06	9.10	M151	2 1 2 2 2	
4.414E-08	8.487E-06	9.14	M183	1 2 1 1 2	

(*continued*)

3421. $C_{15}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.905E-08	9.430E-06	10.80	M063	2 1 2 2 2	
4.900E-08	9.421E-06	10.80	M082	1 1 1 2 2	
4.900E-08	9.421E-06	10.80	M151	2 1 2 2 2	
4.909E-08	9.438E-06	10.84	M183	1 2 1 1 2	
5.773E-08	1.110E-05	13.90	M063	2 1 2 2 2	
5.750E-08	1.106E-05	13.90	M082	1 1 1 2 2	
5.750E-08	1.106E-05	13.90	M151	2 1 2 2 2	
5.778E-08	1.111E-05	13.94	M183	1 2 1 1 2	
7.542E-08	1.450E-05	18.30	M063	2 1 2 2 2	
7.540E-08	1.450E-05	18.30	M082	1 1 1 2 2	
7.540E-08	1.450E-05	18.30	M151	2 1 2 2 2	
7.550E-08	1.452E-05	18.34	M183	1 2 1 1 2	
9.934E-08	1.910E-05	23.10	M063	2 1 2 2 2	
9.940E-08	1.911E-05	23.10	M082	1 1 1 2 2	
9.940E-08	1.911E-05	23.10	M151	2 1 2 2 2	
9.944E-08	1.912E-05	23.14	M183	1 2 1 1 2	
2.028E-07	3.900E-05	25	M064	1 1 2 2 1	
1.108E-07	2.130E-05	25.00	M151	2 1 1 2 2	
1.259E-07	2.420E-05	27.00	M063	2 1 2 2 2	
1.260E-07	2.423E-05	27.00	M082	1 1 1 2 2	
1.260E-07	2.423E-05	27.00	M151	2 1 2 2 2	
1.260E-07	2.423E-05	27.04	M183	1 2 1 1 2	
1.670E-07	3.210E-05	31.10	M063	2 1 2 2 2	
1.670E-07	3.211E-05	31.10	M082	1 1 1 2 2	
1.670E-07	3.211E-05	31.10	M151	2 1 2 2 2	
1.671E-07	3.213E-05	31.14	M183	1 2 1 1 2	

3422. $C_{15}H_{12}$

9-Methylanthracene

RN: 779-02-2 **MP** (°C)**:** 79
MW: 192.26 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-06	2.610E-04	25	M064	1 1 2 2 2	
1.330E-06	2.557E-04	25	M342	1 0 1 1 2	
1.358E-06	2.610E-04	ns	M344	0 0 0 0 2	

3423. $C_{15}H_{12}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid benzyl ester
Benzyl 2,4-dichlorophenoxyacetate
2,4-DBE

RN: 13246-97-4 **MP** (°C)**:**
MW: 311.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.955E-05	1.542E-02	ns	M120	0 0 1 1 2	

3424. $C_{15}H_{12}Cl_2O_3$

Ethanol, 2-(2,4-dicholrophenoxy)-, benzoate
Benzoate, 2-(2,4-dichlorophenoxy)ethyl-
2,4-DEB
RN: 94-83-7 **MP** (°C)**:** 74
MW: 311.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-04	4.800E-02	ns	B185	0 0 0 0 0	

3425. $C_{15}H_{12}I_3NO_4$

Liothyronine
3,3′,5-Triiodothyronine
RN: 6893-02-3 **MP** (°C)**:** 236dec
MW: 650.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.080E-06	3.958E-03	37	L094	2 0 0 1 2	pH 4-5, zwitterion

3426. $C_{15}H_{12}N_2O$

5H-Dibenz[b,f]azepine-5-carboxamide
Carbazepine
5-Carbamoyl-5H-dibenz[b,f]azepine
Iminostilbene
Carbamazepine
Epitol
RN: 298-46-4 **MP** (°C)**:** 190–193
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.655E-04	1.100E-01	20	B196	0 0 0 0 0	
4.700E-04	1.110E-01	20	B196	0 0 0 0 0	
6.349E-04	1.500E-01	25	C437	0 0 0 0 0	Average
1.864E-03	4.404E-01	32	F425	0 0 0 0 0	pH 7.4
1.100E-03	2.600E-01	amb	L434	0 0 0 0 0	
4.232E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.000E-03	9.451E-01	rt	B397	0 0 0 0 0	EFG

3427. $C_{15}H_{12}N_2O_2$

Phenytoin
5,5-Diphenyl-2,4-imidazolidinedione
Dilantin
5,5-Diphenylhydantoin
Ekko
Zentropil

RN: 57-41-0 **MP** (°C)**:** 296.5
MW: 252.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.765E-04	9.499E-02	0	B114	1 1 1 2 1	pH 6-7
1.268E-04	3.200E-02	22	B154	1 1 1 1 1	0.1M HCl
7.531E-05	1.900E-02	25	A408	2 0 1 2 0	int
5.549E-05	1.400E-02	25	P061	0 0 0 0 0	pH 1-7
1.526E-04	3.850E-02	37	F183	1 0 1 1 2	intrinsic
2.600E-04	6.559E-02	50	M335	1 0 2 1 2	pH 5
2.323E-04	5.860E-02	ns	K446	0 0 0 0 0	
7.650E-05	1.930E-02	rt	I404	0 0 0 0 0	Average

3428. $C_{15}H_{12}N_2O_2$

Disperse violet 4
1-Amino-4-(*N*-methylamino)anthraquinone
Interchem acetate violet 6B

RN: 1220-94-6 **MP** (°C)**:** 193
MW: 252.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	5.802E-04	25	B333	0 0 0 0 0	

3429. $C_{15}H_{12}N_2O_3$

5-Phenyl-5-(*p*-hydroxy)phenyl-hydantoin
DL-5-(*p*-Hydroxyphenyl-5-phenylhydantoin
p-Hydroxyphenytoin
Hydroxydiphenylhydantoin
p-Hydroxydiphenylhydantoin

RN: 2784-27-2 **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.342E-04	3.600E-02	37	F183	1 0 1 1 2	intrinsic

3430. $C_{15}H_{12}N_2O_3$

Furfurin
1H-Imidazole, 2,4,5-tri-2-furanyl-4,5-dihydro-
2-Imidazoline, 2,4,5-tri-2-furyl-
RN: 550-23-2 **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.000E-01	8	F300	1 0 0 0 0	
2.870E-02	7.700E+00	100	F300	1 0 0 0 1	

3431. $C_{15}H_{12}O_4$

Benzoyl-*r*-mandelic acid
p-Benzoylmandelic acid
RN: 100915-04-6 **MP** (°C)**:** 177
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-02	5.074E+00	0	A043	1 2 1 1 1	
1.980E-02	5.074E+00	0	L035	1 2 2 1 1	
2.327E-02	5.964E+00	10	A043	1 2 1 1 1	
2.327E-02	5.964E+00	10	L035	1 2 2 1 1	
2.520E-02	6.458E+00	15	A043	1 2 1 1 1	
2.520E-02	6.458E+00	15	L035	1 2 2 1 1	
2.828E-02	7.247E+00	20	A043	1 2 1 1 1	
2.828E-02	7.247E+00	20	L035	1 2 2 1 1	
3.059E-02	7.838E+00	25	A043	1 2 1 1 1	
3.059E-02	7.838E+00	25	L035	1 2 2 1 1	
3.557E-02	9.116E+00	30	A043	1 2 1 1 1	
3.557E-02	9.116E+00	30	L035	1 2 2 1 1	
4.017E-02	1.029E+01	35	A043	1 2 1 1 2	
4.017E-02	1.029E+01	35	L035	1 2 2 1 2	
4.894E-02	1.254E+01	40	A043	1 2 1 1 2	
4.894E-02	1.254E+01	40	L035	1 2 2 1 2	
6.032E-02	1.546E+01	45	A043	1 2 1 1 2	
6.032E-02	1.546E+01	45	L035	1 2 2 1 2	
7.201E-02	1.845E+01	50	A043	1 2 1 1 2	
7.201E-02	1.845E+01	50	L035	1 2 2 1 2	

3432. $C_{15}H_{12}O_4$

Benzoic acid, 2-(acetyloxy)-, phenyl ester
Phennin
Phenyl 2-acetoxybenzoate
Vesipyrin
Spiroform
Phenyl acetylsalicylate

RN: 134-55-4 **MP** (°C)**:** 97.5
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.805E-05	2.000E-02	21	N335	0 0 0 0 0	

3433. $C_{15}H_{13}Cl_3O_2$

2-*p*-Methoxyphenyl-2-*p*-hydroxyphenyl-1,1,1-trichloro-ethane
Phenol, 4-[2,2,2-trichloro-1-(4-methoxyphenyl)ethyl]-

RN: 28463-03-8 **MP** (°C)**:** 112–114
MW: 331.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-06	8.000E-04	ns	K117	0 1 2 1 1	

3434. $C_{15}H_{13}FO_2$

Flurbiprofen
3-Fluoro-4-phenylhydratropic acid
Froben
Ansaid

RN: 5104-49-4 **MP** (°C)**:** 110
MW: 244.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-05	6.180E-03	5	F306	1 0 1 2 2	intrinsic
2.761E-05	6.744E-03	24.99	K447	0 0 0 0 0	pH 2.0
4.339E-05	1.060E-02	25	A408	2 0 1 2 0	int
5.000E-05	1.221E-02	25	A411	1 0 0 1 0	int
1.332E-04	3.254E-02	25	C314	0 0 0 0 0	
1.331E-04	3.250E-02	25	C314	0 0 0 0 0	
3.870E-05	9.453E-03	25	F306	1 0 1 2 2	intrinsic
1.940E-04	4.739E-02	25	O303	1 0 0 1 0	EFG
4.600E-05	1.124E-02	37	F306	1 0 1 2 2	intrinsic
2.866E-05	7.000E-03	37	Y421	0 0 0 0 0	
>2.05E-03	>5.00E-01	ns	B404	0 2 1 1 0	
2.700E-04	6.595E-02	ns	O304	0 0 1 2 2	
3.275E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic

3435. $C_{15}H_{13}F_3N_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methyl-4-(trifluoromethyl)-

RN: 135794-72-8 **MP** (°C)**:**
MW: 322.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.209E-05	2.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3436. $C_{15}H_{13}NO$

7-Benzoylindoline
U-26,952

RN: 33244-57-4 **MP** (°C)**:** 124
MW: 223.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-05	2.290E-03	25	C046	0 0 0 0 0	

3437. $C_{15}H_{13}NO_2$

Dibenz[b,f][1,4]oxazepin-11(10H)-one, 10-ethyl-

RN: 17296-50-3 **MP** (°C)**:**
MW: 239.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.089E-04	4.999E-02	ns	M381	0 1 1 1 2	pH 7.0

3438. $C_{15}H_{13}NO_2S$

Metiazinic acid
Methiazinic acid

RN: 13993-65-2 **MP** (°C)**:** 146
MW: 271.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	3.100E-02	30	D015	2 0 1 1 0	EFG
2.211E-04	6.000E-02	37	D015	2 0 1 1 0	EFG

3439. $C_{15}H_{13}NO_3$

Ketorolac

RN: 74103-06-3 **MP** (°C)**:**
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.167E-04	1.830E-01	32	C411	2 1 1 2 1	
4.309E-04	1.100E-01	37	Y421	0 0 0 0 0	

3440. $C_{15}H_{13}NO_3$

Benzoyl acetaminophen
Acetamide, *N*-[4-(benzoyloxy)phenyl]-
Acetanilide, 4′-hydroxy-, benzoate (ester)
RN: 537-52-0 **MP** (°C)**:** 170.5–171.5
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-05	1.700E-02	37	D029	0 0 0 0 0	

3441. $C_{15}H_{13}NO_4$

Phenyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl phenyl ester
Acetanilide, 4′-hydroxy-, phenyl carbonate (ester)
RN: 17239-23-5 **MP** (°C)**:** 139–140.5
MW: 271.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-04	6.300E-02	37	D029	0 0 0 0 0	

3442. $C_{15}H_{13}N_3O_4S$

Piroxicam
2H-1,2-Benzothiazine-3-carboxamide, 4-hydroxy-2-methyl-*N*-2-pyridinyl-, 1,1-dioxide
Fensaid
Feldene
Candyl
Mobilis
RN: 36322-90-4 **MP** (°C)**:** 198
MW: 331.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-04	8.400E-02	25	M457	0 0 0 0 0	
1.608E-04	5.330E-02	32	C411	2 1 1 2 1	
<3.02E-04	<1.00E-01	rt	B435	0 0 0 0 0	
6.941E-05	2.300E-02	rt	H302	0 0 2 1 2	intrinsic

3443. $C_{15}H_{14}ClN_3O_4S$

Cefaclor
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2*R*)-aminophenylacetyl]amino]-3-chloro-8-oxo-, (6*R*,7*R*)-
Ceclor
Alfacet
Cephaclor
RN: 53994-73-3 **MP** (°C)**:**
MW: 367.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-02	1.000E+01	ns	L099	0 0 0 0 0	

3444. $C_{15}H_{14}ClN_3O_4S_3$

Benzthiazide
Exna
Hydrex
RN: 91-33-8 **MP** (°C)**:**
MW: 431.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.547E-05	1.100E-02	ns	B404	0 2 1 1 0	
6.482E-06	2.800E-03	rt	I404	0 0 0 0 0	Intrinsic, Average

3445. $C_{15}H_{14}Cl_2F_3N_3O_3$

Carfentrazone-ethyl
Df herbicide
Benzenepropanoic acid, α-2-dichloro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}-4-fluoro-, ethyl ester
Ethyl 2-chloro-3-{2-chloro-4-fluoro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}phenyl}propanoate
F 8426
RN: 128639-02-1 **MP** (°C)**:**
MW: 412.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.333E-05	2.198E-02	ns	S460	0 0 0 0 0	

3446. $C_{15}H_{14}Cl_2N_4O_3$
C.I. Disperse orange 5
Ethanol, 2-[[4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]methylamino]
Amacel fast brown 3R
Celliton fast brown 3R
RN: 6232-56-0 **MP** (°C)**:** 127
MW: 369.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-07	1.588E-04	25	B333	0 0 0 0 0	
8.938E-06	3.300E-03	60	P313	0 0 0 0 0	average of 2
1.530E-05	5.650E-03	70	P313	0 0 0 0 0	average of 2
2.939E-05	1.085E-02	80	P313	0 0 0 0 0	average of 2
6.378E-05	2.355E-02	90	P313	0 0 0 0 0	average of 2
1.354E-04	5.000E-02	100	P313	0 0 0 0 0	

3447. $C_{15}H_{14}F_3N_3O_4S_2$
Bendroflumethiazide
Corzide
Rauzide
Naturetin
RN: 73-48-3 **MP** (°C)**:** 222
MW: 421.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	5.057E-02	20	A080	1 0 2 1 2	
2.570E-04	1.083E-01	25	A076	1 0 1 1 2	
2.847E-05	1.200E-02	ns	B404	0 2 1 1 0	
9.492E-05	4.000E-02	rt	A095	0 0 2 2 0	
3.631E-05	1.530E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

3448. $C_{15}H_{14}NO_2PS$
Cyanofenphos
O-(4-Cyanophenyl) *O*-ethyl phenylphosphonothioate
Surecide
RN: 13067-93-1 **MP** (°C)**:** 83
MW: 303.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-06	6.000E-04	30	M161	1 0 0 0 0	

3449. $C_{15}H_{14}N_2O_2$
Dibenz[b,f][1,4]oxazepin-11(10H)-one, 8-amino-2-methyl-
RN: 155206-47-6 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-04	3.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3450. $C_{15}H_{14}N_2O_3$
p-(3-Phenylureido)phenyl acetate
Benzeneacetic acid, 4-[[(phenylamino)carbonyl]amino]-
RN: 181518-40-1 **MP** (°C)**:**
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	9.730E-03	25	A066	1 0 1 1 1	

3451. $C_{15}H_{14}N_2O_5$
2′-Ethoxy-2hydroxy-5-nitrobenzanilide
Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-5-nitro-
RN: 213460-67-4 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-05	5.098E-03	25	D400	2 0 0 1 2	

3452. $C_{15}H_{14}N_2O_5$
4′-Ethoxy-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(4-ethoxyphenyl)-2-hydroxy-3-nitro-
RN: 213460-61-8 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:** 342.2–426.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.119E-05	9.428E-03	25	D400	2 0 0 1 2	

3453. $C_{15}H_{14}N_2O_5$
2′-Ethoxy-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-3-nitro-
RN: 213460-63-0 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-05	7.352E-03	25	D400	2 0 0 1 2	

3454. $C_{15}H_{14}N_4O$
Nevarapine
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-4-methyl
Nevirapine
BI-RG 587
RN: 129618-40-2 **MP** (°C)**:** 248
MW: 266.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-04	1.000E-01	ns	K444	0 0 0 0 0	
6.412E-04	1.708E-01	ns	M381	0 1 1 1 2	pH 7.0

3455. $C_{15}H_{14}O_3$
Methyl benzoyl benzoate
Benzoic acid, 4-hydroxy-, (4-methylphenyl)methyl ester
RN: 84833-58-9 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.064E-04	5.000E-02	ns	F014	0 0 0 0 0	

3456. $C_{15}H_{14}O_3$
[4-(Benzyloxy)phenyl]acetic acid
(4-Boph)
RN: 6547-53-1 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.711E-04	6.568E-02	20	K437	0 0 0 0 0	pH 2.0
3.711E-04	8.990E-02	25	K437	0 0 0 0 0	pH 2.0
6.338E-04	1.536E-01	30	K437	0 0 0 0 0	pH 2.0
7.293E-04	1.767E-01	37	K437	0 0 0 0 0	pH 2.0

3457. $C_{15}H_{14}O_3$
Fenoprofen
Fenoporfen
Progesic
Fenpron
Nalfon
Fenopron
RN: 31879-05-7 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-04	1.000E-01	37	Y421	0 0 0 0 0	

3458. $C_{15}H_{15}ClF_3N_3O$

Triflumizole

RN: 99387-89-0 **MP** (°C)**:** 63.5
MW: 345.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.480E-05	1.549E-02	25	V410	0 0 0 0 0	

3459. $C_{15}H_{15}ClN_2O_2$

Chlorooxuron
(*N′*-4-(4-Chlorophenoxy)phenyl-*N,N*-dimethylurea)
3-[*p*-(*p′*-Chlorophenoxy)phenyl]-1,1-dimethylurea
N-4-(4′-Chlorophenoxy)phenyl-*N′,N′*-dimethylurea
Tenoran

RN: 1982-47-4 **MP** (°C)**:** 151
MW: 290.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-05	3.700E-03	20	B185	0 0 0 0 0	
1.273E-05	3.700E-03	20	G036	1 0 0 0 1	
1.273E-05	3.700E-03	20	M161	1 0 0 0 1	pH 7
9.286E-06	2.700E-03	ns	B200	0 0 0 0 1	
1.273E-04	3.700E-02	ns	M061	0 0 0 0 1	

3460. $C_{15}H_{15}ClN_2O_4S$

Xipamide
2′,6′-Salicyloxylidide, 4-chloro-5-sulfamoyl-
Aquaphor
Aquaphor (diuretic)
BEI 1293
Diurex

RN: 14293-44-8 **MP** (°C)**:** 256
MW: 354.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.635E-04	5.800E-02	25	H074	1 2 2 1 1	

3461. $C_{15}H_{15}ClN_4O_6S$

Chlorimuron-ethyl
Chlorimuron ethyl ester
Classic 75DF
Classic
Chlorimuron Et
2-[[[[(4-Chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]benzoic acid ethyl ester
RN: 90982-32-4 **MP** (°C)**:** 180–182
MW: 414.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.455E-06	1.018E-03	ns	R427	0 0 0 0 0	

3462. $C_{15}H_{15}ClO$

2-Benzyl-3,5-dimethyl-4-chloro-phenol
RN: 1867-85-2 **MP** (°C)**:**
MW: 246.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.234E-02	25	B316	0 0 0 0 0	

3463. $C_{15}H_{15}NO_2$

Mefenamic acid
2′,3′-Dimethyl-*N*-phenyl-anthranilic acid
Forte mefenamic acid
N-(2,3-Xylyl)anthranilic acid
Ponstel
Ponstan
RN: 61-68-7 **MP** (°C)**:** 230.5
MW: 241.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.289E-05	2.000E-02	30	D015	2 0 1 1 0	EFG
2.800E-05	6.756E-03	35	H091	1 2 2 2 1	*sic*
1.658E-04	4.000E-02	37	D015	2 0 1 1 0	EFG
1.658E-06	4.000E-04	37	P432	0 0 0 0 0	
1.227E-04	2.960E-02	37	P432	0 0 0 0 0	
8.289E-07	2.000E-04	37	Y421	0 0 0 0 0	
1.100E-04	2.654E-02	ns	O304	0 0 1 2 2	

3464. $C_{15}H_{15}NO_3$
Tolmetin
Tolectin
RN: 26171-23-3 **MP** (°C)**:**
MW: 257.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-05	2.000E-02	37	Y421	0 0 0 0 0	

3465. $C_{15}H_{15}N_3O$
5H-Pyrido[2,3-b][1,5]benzodiazepine-5-one, 11-ethyl-6,11-dihydro-6-methyl-
RN: 132686-75-0 **MP** (°C)**:**
MW: 253.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.782E-05	4.515E-03	ns	M381	0 1 1 1 2	pH 7.0
4.742E-04	1.201E-01	ns	M381	0 1 1 1 2	pH 7.0

3466. $C_{15}H_{15}N_3O_2$
Pyrido[2,3-b][1,5]benzoxazepin-5(6H)-one, 3-amino-6,7,9-trimethyl-
RN: **MP** (°C)**:**
MW: 269.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	4.658E-02	ns	M381	0 1 1 1 2	pH 7.0

3467. $C_{15}H_{15}N_3O_2$
C.I. Disperse yellow 3
Acetamide, *N*-[4-[(2-hydroxy-5-methylphenyl)azo]phenyl]-
RN: 2832-40-8 **MP** (°C)**:** 195
MW: 269.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.232E-05	25	B333	0 0 0 0 0	

3468. $C_{15}H_{15}N_3S$
5H-Pyrido[2,3-b][1,5]benzodiazepine-5-thione, 11-ethyl-6,11-dihydro-6-methyl-
RN: 132686-95-4 **MP** (°C)**:**
MW: 269.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.968E-05	5.301E-03	ns	M381	0 1 1 1 2	pH 7.0

3469. $C_{15}H_{16}N_2O_2$
Ancymidol
α-Cyclopropyl-α-(4-methoxyphenyl)-5-pyrimidinemethanol
A-Rest
RN: 12771-68-5 **MP** (°C)**:** 110.5
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-03	6.500E-01	25	M161	1 0 0 0 2	

3470. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 5,11-dihydro-5-methyl-11-propyl-
RN: 132312-81-3 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-03	3.562E-01	ns	M381	0 1 1 1 2	pH 7.0

3471. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2,4-dimethyl-
RN: 134698-31-0 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.793E-05	7.493E-03	ns	M381	0 1 1 1 2	pH 7.0

3472. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 5,11-diethyl-5,11-dihydro-
RN: 132312-82-4 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-03	3.704E-01	ns	M381	0 1 1 1 2	pH 7.0

3473. $C_{15}H_{16}N_4O_2$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methoxy-4-methyl-
RN: 135794-75-1 **MP** (°C)**:**
MW: 284.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-06	1.999E-03	ns	M381	0 1 1 1 2	pH 7.0

3474. $C_{15}H_{16}N_4O_2$

1H-Purine-2,6-dione, 1,3-diethyl-3,7-dihydro-8-phenyl-
1,3-Diethyl-8-phenylxanthine
8-Phenyl-1,3-diethylxanthine

RN: 75922-48-4 **MP** (°C)**:**
MW: 284.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.517E-06	1.000E-03	ns	H316	0 0 0 0 0	0.1N HCL
2.110E-05	6.000E-03	ns	H316	0 0 0 0 0	pH 7.4

3475. $C_{15}H_{16}N_4O_5S$

Benzenesulfonic acid, 4-(1,3-Diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-

RN: 89073-47-2 **MP** (°C)**:** >360
MW: 364.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.56E-01	>5.70E+01	ns	H316	0 0 0 0 0	pH 7.4
>2.20E-02	>8.00E+00	ns	H316	0 0 0 0 0	0.1N HCL

3476. $C_{15}H_{16}O_2$

Bisphenol A
2,2-*bis*-[4-Hydroxyphenyl]-propan
2,2-*bis*-(4-Hydroxypheny)-propane

RN: 80-05-7 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.533E-03	3.500E-01	20	F300	1 0 0 0 1	
4.775E-04	1.090E-01	22	Y419	0 0 0 0 0	
1.314E-03	3.000E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	25	D415	1 0 0 0 0	
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	
1.314E-03	3.000E-01	25	S468	0 0 0 0 0	

3477. $C_{15}H_{16}O_2$
Bisphenol A
RN: 80-05-7 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	

3478. $C_{15}H_{16}O_2$
Nabumetone
RN: 42924-53-8 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.628E-05	6.000E-03	22.5	C438	0 0 0 0 0	

3479. $C_{15}H_{16}O_3$
Osthole
2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methyl-2-butenyl)-
RN: 484-12-8 **MP** (°C)**:** 83.5
MW: 244.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.912E-05	1.200E-02	30	B144	1 0 1 0 1	

3480. $C_{15}H_{16}O_9.2H_2O$
Aesculin (dihydrate)
Esculin
6,7-Dihydroxycoumarin 6-glucoside
2H-1-Benzopyran-2-one, 6-(β-D-glucopyranosyloxy)-7-hydroxy-
RN: 531-75-9 **MP** (°C)**:** 205dec
MW: 376.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.605E-03	1.733E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3481. $C_{15}H_{17}FN_4O_2$

Flupirtine

Carbamic acid, [2-amino-6-[[(4-fluorophenyl)methyl]amino]-3-pyridinyl]-, ethyl ester

RN: 56995-20-1 **MP** (°C)**:** 175.8–177.7

MW: 304.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.286E-03	1.000E+00	ns	D321	0 0 0 0 0	

3482. $C_{15}H_{17}NO_3$

Acetamide, 2-(benzoyloxy)-*N,N*-di-acetamide, 2-(benzoyloxy)-*N,N*-di-2-propenyl-

RN: 106231-58-7 **MP** (°C)**:** 42.5

MW: 259.31 **BP** (°C)**:** 401.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.738E-03	7.100E-01	22	B427	1 0 0 1 1	in 0.01M HCl
2.738E-03	7.100E-01	22	N317	1 1 2 1 2	

3483. $C_{15}H_{17}NO_5$

L-Proline, 1-[(benzoyloxy)acetyl]-, methyl ester

RN: 115178-76-2 **MP** (°C)**:** 72.5

MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.239E-03	2.400E+00	22	N317	1 1 2 1 2	

3484. $C_{15}H_{17}NO_7$

Glycine, *N*-[[[2-(acetyloxy)benzoyl]oxy]acetyl]-, ethyl ester

RN: 118247-03-3 **MP** (°C)**:** 68.5

MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.320E+00	21	N335	0 0 0 0 0	

3485. $C_{15}H_{17}N_3O_3S$
L-Ala-dapsone
2-Amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-propanamide
RN: 160348-99-2 **MP** (°C)**:**
MW: 319.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.066E-02	6.600E+00	25	P351	0 0 0 0 0	pH 7.4
>9.39E-02	>3.00E+01	25	P351	0 0 0 0 0	

3486. $C_{15}H_{18}Cl_2N_2O_3$
Oxadiazon
3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one
Ronstar
Scotts OH I
RP-17623
RN: 19666-30-9 **MP** (°C)**:** 88
MW: 345.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-06	7.000E-04	20	M161	1 0 0 0 0	
2.028E-06	7.000E-04	24	C105	2 1 2 2 2	

3487. $C_{15}H_{18}I_3NO_5$
Iopronic acid
Butanoic acid, 2-[[2-[3-(acetylamino)-2,4,6-triiodophenoxy]ethoxy]methyl]-
RN: 37723-78-7 **MP** (°C)**:** 130
MW: 673.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.984E-02	2.008E+01	37	J016	1 0 0 0 2	pH 7.4
1.456E-04	9.799E-02	50	F013	1 0 1 1 1	

3488. $C_{15}H_{18}N_2O_3$
N-Acetyl-L-tryptophan ethyl ester
RN: 2382-80-1 **MP** (°C)**:** 106
MW: 274.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-03	5.200E-01	5	L081	2 2 2 2 1	
5.359E-03	1.470E+00	28	L081	2 1 2 2 2	

3489. $C_{15}H_{18}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-ethyl-5-methylpyrimidine

RN: **MP** (°C)**:**

MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.077E-05	3.600E-03	37	R076	1 2 0 0 1	

3490. $C_{15}H_{18}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-*n*-propylpyrimidine

RN: **MP** (°C)**:**

MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.914E-05	6.400E-03	37	R076	1 2 0 0 2	

3491. $C_{15}H_{18}N_4O_5$

Mitomycin C

MMC

6-Amino-8-[[(aminocarbonyl)oxy]methyl]-1,1α,2,8,8α,8β-hexahydro-8α-methoxy-5-methyl,[1a*S*-(1α,8β,8aα,8bα)]-azirino[2′,3′:3,4]pyrrolo[1,2a]indole-4,7-dione

Mitomycinum

RN: 50-07-7 **MP** (°C)**:** >360

MW: 334.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.730E-03	9.127E-01	25	M316	1 1 1 1 2	
8.500E-01	2.842E+02	ns	B406	0 0 2 2 0	EFG

3492. $C_{15}H_{18}O_3$

Santonin

Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3α,5,5α,9β-tetrahydro-3,5α,9-trimethyl-, (3*S*,3α*S*,5α*S*,9β*S*)-

RN: 481-06-1 **MP** (°C)**:** 170

MW: 246.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-04	2.000E-01	17.5	F300	1 0 0 0 0	
1.624E-02	4.000E+00	100	F300	1 0 0 0 0	

3493. $C_{15}H_{18}O_4$

β-Cyclopentylpropionyl salicylate

RN: **MP** (°C)**:**

MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	2.780E-02	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.91, intrinsic

3494. $C_{15}H_{19}ClO_2$

1,1-Drichloro-1-methyl-2,2-bis(*p*-methoxylphenyl)ethane

RN: 56288-27-8 **MP** (°C)**:**

MW: 266.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-06	1.700E-03	rt	C122	0 0 0 0 0	

3495. $C_{15}H_{19}NO$

N,N-Hexamethylenecinnamamide

Hexahydro-1-(1-oxo-3-phenyl-2-propenyl)1H-azepine

RN: 59832-05-2 **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	5.641E-02	ns	H350	0 0 0 0 0	

3496. $C_{15}H_{19}NO$

N-Cyclohexylcinnamamide

2-Propenamide, *N*-cyclohexyl-3-phenyl-

RN: 6750-98-7 **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-05	9.265E-03	ns	H350	0 0 0 0 0	

3497. $C_{15}H_{19}NO_2$
Tropacocaine
RN: 537-26-8 **MP** (°C)**:** 49
MW: 245.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.055E+00	15	K059	2 2 2 0 1	

3498. $C_{15}H_{19}NO_3$
1H-Azepine, 1-[(benzoyloxy)acetyl]hexahydro-
RN: 115178-68-2 **MP** (°C)**:** 107.5
MW: 261.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E-03	7.500E-01	22	N317	1 1 2 1 2	

3499. $C_{15}H_{19}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(diethylamino)-2-oxoethyl ester
RN: 116482-56-5 **MP** (°C)**:** 76.5
MW: 293.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-03	2.280E+00	21	N335	0 0 0 0 0	

3500. $C_{15}H_{20}N_2O_4$
Benzyl-2,2-diethylmalonurate
Benzyl 2,2-diethylmalonurate

RN: 73632-78-7 **MP** (°C): 107
MW: 292.34 **BP** (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	6.431E-02	23	B152	1 2 1 1 1	pH 3.5

3501. $C_{15}H_{20}N_2O_4S$
Acetohexamide
Acetohexamid
1-(*p*-Acetylbenzenesulfonyl)-3-cyclohexylurea
Dymelor
Dimelin
RN: 968-81-0 **MP** (°C)**:** 189
MW: 324.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.706E-04	2.500E-01	25	K023	1 0 2 2 1	EFG, pH 6.5, average of 2
3.483E-05	1.130E-02	37	B130	1 2 1 1 2	pH 1.5, form II
4.963E-05	1.610E-02	37	B130	1 2 1 1 2	pH 1.5, form III
8.015E-05	2.600E-02	37	K106	1 2 2 2 0	EFG, form I
9.556E-05	3.100E-02	37	K106	1 2 2 2 0	EFG, form II

3502. $C_{15}H_{20}N_4O_2S$
2-Sulfanilylamino-4-amylpyrimidine
RN: 107203-72-5 **MP** (°C)**:**
MW: 320.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-04	2.000E-01	37	R076	1 2 0 0 1	

3503. $C_{15}H_{20}N_4O_5$
1,5-Dibutyryloxymethyl allopurinol
RN: 98827-19-1 **MP** (°C)**:** 122–123
MW: 336.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-04	5.000E-02	22	B322	0 0 0 0 0	

3504. $C_{15}H_{20}N_4O_5$
2,5-Dibutyryloxymethyl allopurinol
RN: 98827-20-4 **MP** (°C)**:** 133–135
MW: 336.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.795E-04	9.400E-02	22	B322	0 0 0 0 0	

3505. $C_{15}H_{20}N_4O_6$
9-[5-*O*-(Butyrate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine
RN: 121032-41-5 **MP** (°C)**:** 108–110
MW: 352.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.680E-03	3.411E+00	37	M378	1 2 1 1 2	pH 7.2

3506. $C_{15}H_{20}N_4O_6.0.3H_2O$
2′-Butyryl-6-methoxypurine arabinoside (0.3 hydrate)
RN: 121032-41-5 **MP** (°C)**:**
MW: 357.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-01	8.264E+01	37	C348	0 0 0 0 0	pH 7.00

3507. $C_{15}H_{20}N_4O_6$
2′-Isobutyryl-6-methoxypurine arabinoside
RN: 121032-44-8 **MP** (°C)**:**
MW: 352.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	2.361E+02	37	C348	0 0 0 0 0	pH 7.00

3508. $C_{15}H_{20}N_4O_6.0.25H_2O$
9-[5-*O*-(Isobutyrate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)
RN: 121032-44-8 **MP** (°C)**:** glass
MW: 356.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	1.367E+01	37	M378	1 2 1 1 2	pH 7.2

3509. $C_{15}H_{21}NO$
N,N-Dipropylcinnamamide
Cinnamamide, *N,N*-dipropyl-
RN: 23784-56-7 **MP** (°C)**:**
MW: 231.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.890E-03	6.686E-01	ns	H350	0 0 0 0 0	

3510. $C_{15}H_{21}NO_2$
Meperidine
Ethyl 1-methyl-4-phenylpiperidine-4-carboxylate
Demerol
Dolantin
Pethidine
RN: 57-42-1 **MP** (°C)**:** 30
MW: 247.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.648E-02	6.550E+00	25	R338	0 0 0 0 0	
1.300E-02	3.215E+00	30	L068	1 0 0 1 0	EFG

3511. $C_{15}H_{21}NO_2S_2$
2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dithiolane
RN: 35801-67-3 **MP** (°C)**:**
MW: 311.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	7.787E-03	rt	B174	0 0 1 0 1	

3512. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-bis(1-methylethyl)-
RN: 106231-56-5 **MP** (°C)**:** 105.5
MW: 263.34 **BP** (°C)**:** 391.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.557E-04	1.200E-01	22	B427	1 0 0 1 1	in 0.01M HCl
4.557E-04	1.200E-01	22	N317	1 1 2 1 2	

3513. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-hexyl-
RN: 115193-29-8 **MP** (°C)**:** 130.5
MW: 263.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	3.300E-02	22	N317	1 1 2 1 2	

3514. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-dipropyl-
RN: 106231-55-4 **MP** (°C)**:** 20
MW: 263.34 **BP** (°C)**:** 402.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.177E-03	1.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.177E-03	1.100E+00	22	N317	1 1 2 1 2	

3515. $C_{15}H_{21}NO_3S$

2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-oxathiolane

RN: 24606-94-8 **MP** (°C)**:**
MW: 295.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.772E-02	rt	B174	0 0 1 0 0	

3516. $C_{15}H_{21}NO_4$

Metalaxyl
Methyl *N*-(2,6-dimethyl-phenyl)-*N*-(2′-methoxyacetyl)-DL-alaninate
Apron
Ridomil
Subdue
Fubol

RN: 57837-19-1 **MP** (°C)**:** 72
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.951E+00	20	E048	1 2 1 1 2	

3517. $C_{15}H_{21}NO_4$

Hexyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl hexyl ester
Acetanilide, 4′-hydroxy-, hexyl carbonate (ester)

RN: 17239-22-4 **MP** (°C)**:** 112.5-113.5
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-04	3.700E-02	37	D029	0 0 0 0 0	

3518. $C_{15}H_{21}NO_4$

2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dioxolane

RN: 35858-24-3 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.514E-01	rt	B174	0 0 1 0 0	

3519. $C_{15}H_{21}NO_5$

Acetamide, 2-(benzoyloxy)-*N,N*-bis(2-methoxyethyl)-

RN: 115178-64-8 **MP** (°C)**:** 57.5
MW: 295.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-02	7.890E+00	22	N317	1 1 2 1 2	

3520. $C_{15}H_{21}NO_5$
Acetamide, 2-(benzoyloxy)-*N*,*N*-bis(2-hydroxypropyl)-
RN: 115178-63-7 **MP** (°C)**:** 105.5
MW: 295.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.636E-02	1.960E+01	22	N317	1 1 2 1 2	

3521. $C_{15}H_{21}N_2O_3$
C.I. Disperse red 11
RN: 2872-48-2 **MP** (°C)**:** 242
MW: 277.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	6.934E-04	25	B333	0 0 0 0 0	

3522. $C_{15}H_{21}N_3O$
Primaquine
Primaquine phosphate
Neo-quipenyl
8-(4-Amino-1-methylbutylamino)-6-methoxyquinoline
8-((4-Amino-1-methylbutyl)amino)-6-methoxyquinoline phosphate
Palum
RN: 90-34-6 **MP** (°C)**:**
MW: 259.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.770E+00	7.184E+02	25	B443	0 0 0 0 0	

3523. $C_{15}H_{21}N_5O_5$
9-(2-*O*-Valeryl-β-D-arabinofuranosyl)adenine
RN: 87984-85-8 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.960E-04	1.040E-01	37	B306	1 2 0 1 2	pH 7.3

3524. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Isovaleryl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-32-1 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	1.980E+01	ns	B134	0 1 1 1 2	

3525. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Valeryl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-31-0 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.391E-02	8.400E+00	ns	B134	0 1 1 1 1	

3526. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Pivaloyl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-33-2 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-02	7.000E+00	ns	B134	0 1 1 1 1	

3527. $C_{15}H_{21}N_5O_6$
9-(1,3-Dipropionate-2-propoxymethyl)guanine
RN: 86357-20-2 **MP** (°C)**:** 192
MW: 367.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.622E-03	2.800E+00	25	B360	0 0 0 0 0	

3528. $C_{15}H_{22}ClNO_2$
Metolachlor
2-Chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide
Dual
Cotoran Multi
Ontrack 8E
Bicep 6L
RN: 51218-45-2 **MP** (°C)**:** <25
MW: 283.80 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.867E-03	5.297E-01	20	E048	1 2 1 1 2	
1.868E-03	5.300E-01	20	M161	1 0 0 0 2	
1.866E-03	5.297E-01	ns	S460	0 0 0 0 0	
1.868E-03	5.300E-01	ns	V414	0 0 0 0 0	

3529. $C_{15}H_{22}ClNO_2$

CP 52223
2-Chloro-*N*-(2,6-dimethyl)phenyl-*N*-isopropoxymethylacetamide
RN: 24353-58-0 **MP** (°C)**:**
MW: 283.80 **BP** (°C)**:** 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E-04	5.900E-02	ns	M061	0 0 0 0 1	

3530. $C_{15}H_{22}N_2O$

DL-Mepivacaine
Carbocaine
1-Methyl-2′,6′-pipecoloxylidide
Carbocain
RN: 96-88-8 **MP** (°C)**:** 150
MW: 246.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	3.350E+00	14.9	N046	2 0 1 1 1	intrinsic
3.653E-02	9.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
2.841E-02	7.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
9.000E-03	2.217E+00	25	D402	1 2 2 2 0	EFG
1.020E-02	2.513E+00	25	N046	2 0 1 1 1	intrinsic
9.910E-03	2.441E+00	34.5	N046	2 0 1 1 1	intrinsic
1.000E-02	2.464E+00	37	D402	1 2 2 2 0	EFG
7.970E-03	1.963E+00	37	N044	2 1 1 2 2	intrinsic

3531. $C_{15}H_{22}O_3$

Gemfibrozil
2,2-Dimethyl-5-(2,5-xylyloxy)valeric acid
Jezil
Lobid
Lopid
RN: 25812-30-0 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.00E-03	>5.00E-01	ns	B404	0 2 1 1 0	

3532. $C_{15}H_{22}O_3$

Octyl *p*-hydroxybenzoate
n-Octyl 4-hydroxybenzoate
RN: 1219-38-1 **MP** (°C)**:** 54
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-05	3.680E-03	15	B355	0 0 0 0 0	
2.300E-04	5.758E-02	20	B355	0 0 0 0 0	
4.650E-04	1.164E-01	25	B355	0 0 0 0 0	
3.273E-03	8.193E-01	25	D081	1 2 2 1 2	
3.162E-04	7.916E-02	25	F322	2 0 1 1 0	EFG

3533. $C_{15}H_{22}O_5$

Octyl gallate
Octyl 3,4,5-trihydroxybenzoate
n-Octyl gallate
RN: 1034-01-1 **MP** (°C)**:**
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.084E-05	2.000E-02	29.99	L430	0 0 0 0 0	
8.500E-05	2.400E-02	34.99	L430	0 0 0 0 0	
1.133E-04	3.200E-02	39.99	L430	0 0 0 0 0	
1.806E-04	5.100E-02	44.99	L430	0 0 0 0 0	
3.152E-04	8.899E-02	49.99	L430	0 0 0 0 0	
4.214E-04	1.190E-01	54.99	L430	0 0 0 0 0	
4.710E-04	1.330E-01	59.99	L430	0 0 0 0 0	
5.064E-04	1.430E-01	64.99	L430	0 0 0 0 0	

3534. $C_{15}H_{23}NO_2$

Octyl *m*-aminobenzoate
Octyl 3-aminobenzoate
RN: 52222-35-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	7.481E-03	ns	M066	0 0 0 0 0	

3535. $C_{15}H_{23}NO_2$

Octyl *p*-aminobenzoate
4-Aminobenzoic acid octyl ester
RN: 14309-41-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-06	7.979E-04	37	F006	1 1 2 2 1	

3536. $C_{15}H_{23}NO_2$

Alprenolol
Aptin
RN: 13655-52-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.471E-03	3.669E-01	22.5	B422	0 0 0 0 0	

3537. $C_{15}H_{23}NO_3$

Parethoxycaine
4-Ethoxybenzoic acid-2-(diethylamino)ethyl ester
RN: 94-23-5 **MP** (°C)**:** 173.0
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-03	5.121E-01	ns	M066	0 0 0 0 2	

3538. $C_{15}H_{23}NO_4$

Cycloheximide
3-((*R*)-2-((1*S*,3*S*,5*S*)-3,5-Dimethyl-2-oxocyclohexyl)-2-hydroxyethyl)glutarimide
Actidione
Actispray
Naramycin
Kaken
RN: 66-81-9 **MP** (°C)**:** 116.3
MW: 281.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.464E-02	2.100E+01	2	M161	1 0 0 0 1	

3539. $C_{15}H_{23}N_3O_4$

Isopropalin
2,6-Dinitro-*N,N*-dipropylcumidene
4-Isopropyl-2,6-dinitro-*N,N*-dipropylaniline
2,6-Dinitro-*N,N*-dipropylcumidine
Paarlan
Paarlan EC
RN: 33820-53-0 **MP** (°C)**:**
MW: 309.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.232E-07	1.000E-04	25	M161	1 0 0 0 0	

3540. $C_{15}H_{23}N_3O_4S$

Sulpiride

N-[(1-Ethyl-2-pyrrolidinyl)methyl]-2-methoxy-5-sulfamoylbenzamide

RN: 15676-16-1 **MP** (°C)**:**

MW: 341.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-04	<2.10E-01	25	P312	0 0 0 0 0	

3541. $C_{15}H_{23}N_3O_4S$

Cyclacillin

Anhydrous 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 **MP** (°C)**:**

MW: 341.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-01	5.500E+01	7	P035	0 0 0 0 0	EFG
1.054E-01	3.600E+01	20	P035	0 0 0 0 0	EFG
9.372E-02	3.200E+01	25	P035	0 0 0 0 0	EFG
7.908E-02	2.700E+01	30	P035	0 0 0 0 0	EFG
6.736E-02	2.300E+01	40	P035	0 0 0 0 0	EFG
6.151E-02	2.100E+01	50	P035	0 0 0 0 0	EFG
5.858E-02	2.000E+01	60	P035	0 0 0 0 0	EFG

3542. $C_{15}H_{23}N_3O_4S.2H_2O$

Cyclacillin (dihydrate)

Dihydrate 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 **MP** (°C)**:**

MW: 377.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	1.400E+01	10	P035	0 0 0 0 0	EFG
3.709E-02	1.400E+01	20	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	25	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	30	P035	0 0 0 0 0	EFG
3.682E-02	1.390E+01	40	P035	0 0 0 0 0	EFG
3.762E-02	1.420E+01	50	P035	0 0 0 0 0	EFG
4.504E-02	1.700E+01	60	P035	0 0 0 0 0	EFG

3543. $C_{15}H_{24}NO_4PS$

Isofenphos
Methylethyl 2-((ethoxy((1-methylethyl)amino)phosphinothioyl)oxy)benzoate
Amaze
Oftanol
Pryfon
RN: 25311-71-1 **MP** (°C)**:**
MW: 345.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-05	2.210E-02	20	B300	2 1 1 1 2	*sic*
6.891E-02	2.380E+01	20	M161	1 0 0 0 2	*sic*

3544. $C_{15}H_{24}N_2O_2$

N,N,N′-Triethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide
RN: 62249-37-0 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-01	5.900E+01	20	K050	1 1 1 1 2	

3545. $C_{15}H_{24}N_2O_2$

Tetracaine
Pantocaine
Cetacaine
RN: 94-24-6 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	1.560E-01	ns	E031	0 0 2 1 2	

3546. $C_{15}H_{24}N_2O_2$

4-Ethylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-53-2 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-03	1.216E+00	ns	M066	0 0 0 0 1	

3547. $C_{15}H_{24}N_2O_2$

4-Aminobenzoic acid-2-(diethyl-amino)butyl ester
2-(Diethyl(amino)butyl 4-aminobenzoate
RN: 5878-14-8 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.137E+00	ns	M066	0 0 0 0 1	

3548. $C_{15}H_{24}N_2O_3$

2,4-Diazaspiro[5.11]heptadecane-1,3,5-trione
RN: 143288-64-6 **MP** (°C)**:**
MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-06	4.486E-04	25	P350	0 0 0 0 0	intrinsic

3549. $C_{15}H_{24}O$

Butylated hydroxytoluene
2,6-Di-*tert*-butyl-*p*-cresol
2,6-Di-*tert*-butyl-1-hydroxy-4-methylbenzene
4-Hydroxy-3,5-di-*tert*-butyltoluene
RN: 128-37-0 **MP** (°C)**:** 71
MW: 220.36 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.54E-05	<1.00E-02	25	P312	0 0 0 0 0	

3550. $C_{15}H_{24}O$

4-Nonylphenol
4-*t*-Nonylphenol
RN: 104-40-5 **MP** (°C)**:**
MW: 220.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-05	4.605E-03	2	A335	0 0 0 0 0	
2.088E-05	4.600E-03	2	A335	0 0 0 0 0	
2.230E-05	4.914E-03	10	A335	0 0 0 0 0	
2.233E-05	4.920E-03	10	A335	0 0 0 0 0	
2.380E-05	5.245E-03	14	A335	0 0 0 0 0	
2.378E-05	5.240E-03	14	A335	0 0 0 0 0	
2.470E-05	5.443E-03	20.5	A335	0 0 0 0 0	
2.464E-05	5.430E-03	20.5	A335	0 0 0 0 0	
2.882E-05	6.350E-03	25	A335	0 0 0 0 0	
2.890E-05	6.368E-03	25	A335	0 0 0 0 0	
3.177E-05	7.000E-03	25	M127	1 0 0 0 0	

3551. $C_{15}H_{24}O$

Nonylphenol

RN: 25154523 **MP** (°C)**:**
MW: 220.36 **BP** (°C)**:** 293–297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.224E-05	4.900E-03	25	B420	1 1 1 1 1	

3552. $C_{15}H_{26}N_2$

Sparteine
(–)-Spartein

RN: 90-39-1 **MP** (°C)**:** 30
MW: 234.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.297E-02	3.040E+00	22	F300	1 0 0 0 2	
1.297E-02	3.040E+00	25	D004	0 0 0 0 0	

3553. $C_{15}H_{26}N_2O_3$

5-Allyl-5-methylhexylcarbinylbarbituric acid

RN: **MP** (°C)**:**
MW: 282.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	3.060E+00	ns	T003	0 0 0 0 2	

3554. $C_{15}H_{26}N_2O_3$

5-Ethyl-5-*n*-nonylbarbituric acid
5-Ethyl-5-nonylbarbiturate

RN: 64810-91-9 **MP** (°C)**:**
MW: 282.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	9.742E-02	25	M310	2 2 2 2 2	

3555. $C_{15}H_{26}O_6$

Tributyrin
Glyceryl tributyrate
Tributanoylglycerol
1,2,3-Propanetriyl tributyrate

RN: 60-01-5 **MP** (°C)**:** 173
MW: 302.37 **BP** (°C)**:** 287.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-04	9.999E-02	ns	F014	0 0 0 0 1	

3556. $C_{15}H_{28}O_4$
1,13-Tridecanedicarboxylic acid
1,15-Pentadecandioic acid
RN: 1460-18-0 **MP** (°C)**:**
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-03	3.500E-01	21	B040	1 0 1 1 1	*sic*

3557. $C_{15}H_{30}$
1-Pentadecene
RN: 13360-61-7 **MP** (°C)**:**
MW: 210.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E-09	3.740E-07	23	C332	0 0 0 0 0	

3558. $C_{15}H_{30}O_2$
Pentadecylic acid
Pentadecanoic acid
RN: 1002-84-2 **MP** (°C)**:** 52
MW: 242.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.135E-05	7.600E-03	0	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20.0	R001	1 1 1 1 1	
5.775E-05	1.400E-02	30	B136	1 0 2 1 1	
5.775E-05	1.400E-02	30.0	R001	1 1 1 1 1	
7.013E-05	1.700E-02	45	B136	1 0 2 1 1	
7.013E-05	1.700E-02	45.0	R001	1 1 1 1 1	
8.251E-05	2.000E-02	60	B136	1 0 2 1 1	
8.250E-05	2.000E-02	60.0	R001	1 1 1 1 1	
3.135E-05	7.600E-03	.0	R001	1 1 1 1 1	

3559. $C_{15}H_{30}O_3$
Dodecyl lactate
Propanoic acid, 2-hydroxy-, dodecyl ester
RN: 6283-92-7 **MP** (°C)**:**
MW: 258.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-04	1.000E-01	25	R006	2 2 0 1 0	

3560. $C_{15}H_{32}$

Pentadecane
n-Pentadecane
Pentadecane-d32
Pentadecane (*n*)

RN: 629-62-9 **MP** (°C)**:** 9.9
MW: 212.42 **BP** (°C)**:** 270.63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.883E-10	4.000E-08	25	T423	0 0 0 0 0	

3561. $C_{15}H_{32}O$

Pentadecanol
Pentadecan-1-ol
1-Pentadecanol

RN: 629-76-5 **MP** (°C)**:** 46
MW: 228.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-07	1.028E-04	25	R002	0 0 0 0 0	

3562. $C_{16}H_8Cl_2F_6N_2O_3$

Hexaflumuron

RN: 86479-06-3 **MP** (°C)**:**
MW: 461.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-08	1.620E-05	20	M402	0 0 0 0 0	

3563. $C_{16}H_{10}$

Fluoranthene
1,2-Benzacenaphthene
1,2-(1,8-Naphthalenediyl)benzene
Benzo[j,k]fluorene
Idryl
FA

RN: 206-44-0 **MP** (°C)**:** 107
MW: 202.26 **BP** (°C)**:** 384

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-07	8.191E-05	8.10	M082	1 1 1 2 2	
4.050E-07	8.191E-05	8.10	M151	2 1 2 2 2	
4.058E-07	8.207E-05	8.14	M183	1 1 1 1 2	
5.290E-07	1.070E-04	13.20	M082	1 1 1 2 2	
5.290E-07	1.070E-04	13.20	M151	2 1 2 2 2	

(*continued*)

3563. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.295E-07	1.071E-04	13.24	M183	1 1 1 1 2	
7.330E-07	1.483E-04	19.70	M082	1 1 1 2 2	
7.330E-07	1.483E-04	19.70	M151	2 1 2 2 2	
7.339E-07	1.484E-04	19.74	M183	1 2 1 1 2	
1.190E-06	2.407E-04	20	E009	1 0 0 1 2	
9.394E-07	1.900E-04	20	H300	1 1 2 2 1	
8.850E-07	1.790E-04	20	V416	0 0 0 0 0	
5.933E-07	1.200E-04	24	H116	2 1 0 0 2	
1.000E-06	2.023E-04	24.60	M082	1 1 1 2 2	
1.000E-06	2.023E-04	24.60	M151	2 1 2 2 2	
1.003E-06	2.028E-04	24.64	M183	1 2 1 1 2	
1.400E-06	2.832E-04	25	A325	2 1 2 2 1	
1.023E-06	2.070E-04	25	D406	1 2 2 2 2	
1.320E-06	2.670E-04	25	K001	2 2 2 2 2	
1.335E-06	2.700E-04	25	L332	1 1 1 1 2	
1.285E-06	2.600E-04	25	M064	1 1 2 2 1	
1.019E-06	2.060E-04	25	M071	2 2 2 2 2	
1.300E-06	2.629E-04	25	M342	1 0 1 1 1	
1.167E-06	2.360E-04	25	S227	1 2 1 1 2	
1.019E-06	2.060E-04	25.00	M151	2 1 1 2 2	
1.187E-06	2.400E-04	27	D003	1 0 0 1 1	
1.305E-06	2.640E-04	29	M071	2 2 2 2 2	
1.305E-06	2.640E-04	29.00	M151	2 1 1 2 2	
1.380E-06	2.791E-04	29.90	M082	1 1 1 2 2	
1.380E-06	2.791E-04	29.90	M151	2 1 2 2 2	
1.382E-06	2.796E-04	29.94	M183	1 2 1 1 2	
2.947E-06	5.960E-04	40	V416	0 0 0 0 0	
8.464E-06	1.712E-03	60	V416	0 0 0 0 0	
1.300E-06	2.630E-04	ns	I332	0 0 0 0 1	

3564. $C_{16}H_{10}$

Pyrene

Benzo[def]phenanthrene

RN: 129-00-0 **MP** (°C)**:** 156

MW: 202.26 **BP** (°C)**:** 404

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-07	<2.02E-05	4	K049	1 2 1 1 0	
2.430E-07	4.915E-05	4.70	M082	1 1 1 2 2	
2.430E-07	4.915E-05	4.70	M151	2 1 2 2 2	
2.434E-07	4.924E-05	4.74	M183	1 2 1 1 2	
2.890E-07	5.845E-05	9.50	M082	1 1 1 2 2	
2.890E-07	5.845E-05	9.50	M151	2 1 2 2 2	
2.895E-07	5.855E-05	9.54	M183	1 2 1 1 2	
3.560E-07	7.200E-05	14.30	M082	1 1 1 2 2	
3.560E-07	7.200E-05	14.30	M151	2 1 2 2 2	
3.563E-07	7.206E-05	14.34	M183	1 2 1 1 2	

(*continued*)

3564. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-07	7.258E-05	15	B385	0 0 0 0 0	
4.610E-07	9.324E-05	18.70	M082	1 1 1 2 2	
4.610E-07	9.324E-05	18.70	M151	2 1 2 2 2	
4.617E-07	9.338E-05	18.74	M183	1 2 1 1 2	
5.200E-07	1.052E-04	20	E009	1 0 0 0 1	
5.200E-07	1.052E-04	20	E025	1 0 1 2 1	
4.700E-07	9.506E-05	20	H306	1 0 1 2 1	
5.370E-07	1.086E-04	21.20	M082	1 1 1 2 2	
5.370E-07	1.086E-04	21.20	M151	2 1 2 2 2	
5.394E-07	1.091E-04	21.24	M183	1 2 1 1 2	
7.200E-07	1.456E-04	22	A413	2 0 2 2 1	
6.279E-07	1.270E-04	22.20	W003	2 1 2 2 2	average of 3
6.675E-07	1.350E-04	24	H106	1 0 2 2 2	
1.582E-07	3.200E-05	24	H116	2 1 0 0 1	
6.675E-07	1.350E-04	24	M129	1 2 1 1 2	
5.834E-07	1.180E-04	25	B319	2 0 1 2 2	
6.490E-07	1.313E-04	25	B385	0 0 0 0 0	
7.700E-07	1.557E-04	25	K001	1 0 2 1 2	
4.700E-07	9.506E-05	25	K123	1 0 2 2 1	
7.911E-07	1.600E-04	25	L332	1 1 1 1 2	
6.675E-07	1.350E-04	25	M064	1 1 2 2 2	
6.526E-07	1.320E-04	25	M071	2 2 2 2 2	
6.675E-07	1.350E-04	25	M156	1 2 1 1 2	
6.670E-07	1.349E-04	25	M342	1 0 1 1 2	
3.955E-07	8.000E-05	25	P340	0 0 0 0 0	
3.556E-08	7.191E-06	25	R084	2 2 2 2 1	*sic*
7.400E-07	1.497E-04	25	R302	1 2 1 2 1	
8.455E-07	1.710E-04	25	S227	1 2 1 1 2	
6.526E-07	1.320E-04	25.00	M151	2 1 1 2 2	
6.730E-07	1.361E-04	25.50	M082	1 1 1 2 2	
6.730E-07	1.361E-04	25.50	M151	2 1 2 2 2	
6.728E-07	1.361E-04	25.54	M183	1 2 1 1 2	
8.158E-07	1.650E-04	27	D003	1 0 0 1 1	
8.010E-07	1.620E-04	29	M071	2 2 2 2 2	
8.010E-07	1.620E-04	29.00	M151	2 1 1 2 2	
8.390E-07	1.697E-04	29.90	M082	1 1 1 2 2	
8.390E-07	1.697E-04	29.90	M151	2 1 2 2 2	
8.411E-07	1.701E-04	29.94	M183	1 2 1 1 2	
1.147E-06	2.320E-04	34.50	W003	2 1 2 2 2	average of 2
9.888E-07	2.000E-04	35	B385	0 0 0 0 0	
1.973E-06	3.990E-04	44.70	W003	2 1 2 2 2	average of 3
2.784E-06	5.630E-04	50.10	W003	2 1 2 2 2	average of 3
3.758E-06	7.600E-04	55.60	W003	2 1 2 2 1	average of 3
3.659E-06	7.400E-04	56.00	W003	2 1 2 2 1	
4.648E-06	9.400E-04	60.70	W003	2 1 2 2 1	average of 3
6.329E-06	1.280E-03	65.20	W003	2 1 2 2 2	average of 2
9.196E-06	1.860E-03	71.90	W003	2 1 2 2 2	average of 3
1.093E-05	2.210E-03	74.70	W003	2 1 2 2 2	
6.675E-07	1.350E-04	ns	H123	0 0 0 0 0	

(*continued*)

3564. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.675E-07	1.350E-04	ns	K304	0 0 0 0 2	
6.675E-07	1.350E-04	ns	M344	0 0 0 0 2	
5.000E-07	1.011E-04	ns	M383	0 2 1 1 0	
1.000E-06	2.023E-04	ns	W005	0 0 1 2 0	

3565. $C_{16}H_{10}N_2O_8S_2$

C.I. Acid blue 74(free acid)
Indigo-disulfosaeure-(5,5′)
Indigotinsulfonic acid
RN: 860-22-0 **MP** (°C)**:**
MW: 422.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.37E-02	~1.00E+01	25	F300	1 0 0 0 0	

3566. $C_{16}H_{11}NO_2$

Cinchophen
2-Phenyl-4-quinolinecarboxylic acid
2-Phenylcinchoninic acid
RN: 132-60-5 **MP** (°C)**:** 213
MW: 249.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-04	1.600E-01	25	L074	2 2 1 1 2	

3567. $C_{16}H_{12}F_3NO$

6H-Dibenz[b,e]azepin-6-one, 5,11-dihydro-5-(2,2,2-trifluoroethyl)-
RN: 155206-49-8 **MP** (°C)**:**
MW: 291.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.589E-05	4.627E-03	ns	M381	0 1 1 1 2	pH 7.0

3568. $C_{16}H_{12}N_2O_3$

5,5-Diphenylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diphenyl
Barbituric acid, 5,5-diphenyl
5,5-Diphenylbarbiturate
RN: 21914-07-8 **MP** (°C)**:**
MW: 280.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-05	1.785E-02	25	P350	0 0 0 0 0	intrinsic

3569. $C_{16}H_{12}N_2O_4S$

Sulfanaphthoquinone

RN: **MP** (°C)**:**
MW: 328.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	4.500E-02	20	F073	1 2 2 2 1	

3570. $C_{16}H_{12}O_6$

Hematein
Haematein
Benz[b]indeno[1,2-d]pyran-9(6H)-one, 6α,7-dihydro-3,4,6α,10-tetrahydroxy-

RN: 475-25-2 **MP** (°C)**:** >200
MW: 300.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	6.000E-01	20	F300	1 0 0 0 1	

3571. $C_{16}H_{12}O_6$

Benzoic acid, 2-(acetyloxy)-, 2-carboxyphenyl ester

RN: 530-75-6 **MP** (°C)**:** 166.5
MW: 300.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.661E-05	2.000E-02	21	N335	0 0 0 0 0	

3572. $C_{16}H_{13}ClN_2O$

Diazepam
7-Chloro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
Valium
Valrelease
Vazepam
Diazemuls

RN: 439-14-5 **MP** (°C)**:** 125
MW: 284.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-04	4.200E-02	20	N059	2 0 2 2 2	average of 2
1.756E-04	5.000E-02	25	G084	2 0 2 2 1	
1.756E-04	5.000E-02	25	G095	2 1 2 2 1	
1.756E-04	5.000E-02	25	M159	1 0 2 2 0	EFG, pH 7.0
2.320E-04	6.606E-02	25	M320	2 2 1 1 2	
1.089E-04	3.100E-02	25	M457	0 0 0 0 0	
1.510E-04	4.300E-02	25	N055	2 0 2 2 1	
1.580E-04	4.500E-02	25	N055	2 0 2 1 2	

(*continued*)

3572. $C_{16}H_{13}ClN_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.721E-04	4.900E-02	25	N055	2 0 2 1 2	
1.405E-04	4.000E-02	30	R081	1 2 2 2 0	
2.900E-04	8.258E-02	50	M335	1 0 2 1 2	pH 6.0
1.200E-04	3.417E-02	ns	F327	0 0 1 2 2	
3.512E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.756E-04	5.000E-02	ns	M036	0 0 0 0 0	

3573. $C_{16}H_{13}Cl_2NO_4$

Aceclofenac

RN: 89796-99-6 **MP** (°C)**:**

MW: 354.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.034E-05	3.200E-02	32	C411	2 1 1 2 1	

3574. $C_{16}H_{13}I_3N_2O_3$

Iobenzamic acid

N-(3-Amino-2,4,6-triiodobenzoyl)-*N*-phenyl-β-alanine

Orbil

Osbiland

Razebil

Osbil

RN: 3115-05-7 **MP** (°C)**:**

MW: 662.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	1.150E-01	ns	H055	0 0 0 0 0	

3575. $C_{16}H_{13}NO_3$

C.I. Disperse red 3

N-(2-Hydroxyethyl)-1-aminoanthraquinone

Disperse red 3

Disperse red 66

RN: 4465-58-1 **MP** (°C)**:** 168

MW: 267.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	4.277E-03	25	B333	0 0 0 0 0	

3576. $C_{16}H_{13}N_3$

Yellow AB
1-Phenylazo-2-naphthylamine
RN: 85-84-7 **MP** (°C)**:** 102
MW: 247.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.213E-06	3.000E-04	37	H120	1 1 1 1 0	normal saline

3577. $C_{16}H_{13}N_3O_3$

Mebendazole
Methyl 5-benzoyl benzimidazole-2-carbamate
Pantelmin
Methyl 5-benzoyl-2-benzimidazolecarbamate
RN: 31431-39-7 **MP** (°C)**:** 288.5
MW: 295.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-06	5.000E-04	21	N337	0 0 0 0 0	pH 5
1.700E-06	5.020E-04	21	N337	0 0 0 0 0	pH 5
1.199E-04	3.540E-02	25	H075	1 0 2 1 2	polymorph C
2.414E-04	7.130E-02	25	H075	1 0 2 1 2	polymorph B
3.332E-05	9.840E-03	25	H075	1 0 2 1 2	polymorph A
3.725E-06	1.100E-03	288.5	D426	0 0 0 0 0	
1.318E-04	3.893E-02	ns	R427	0 0 0 0 0	

3578. $C_{16}H_{14}$

9,10-Dimethylanthracene
RN: 781-43-1 **MP** (°C)**:** 182
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-07	5.600E-05	25	M064	1 1 2 2 1	
2.700E-07	5.570E-05	25	M342	1 0 1 1 1	
2.715E-07	5.600E-05	ns	M344	0 0 0 0 2	

3579. $C_{16}H_{14}ClN_3O$

Chlordiazepoxide
7-Chloro-2-(methylamino)-5-phenyl-3H-1,4-benzodiazepine-4-oxide
Librium
Menrium
Tropium
SK-Lygen

RN: 58-25-3 **MP** (°C)**:** 236
MW: 299.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.607E-03	1.981E+00	ns	R427	0 0 0 0 0	
6.672E-03	2.000E+00	rt	M035	0 0 0 0 0	

3580. $C_{16}H_{14}Cl_2N_2O_2$

Phenobenzuron
Benzoyl-1-(3,4-dichlorophenyl)-3,3-dimethylurea
Benzomarc
Urea, *N*-benzoyl-*N*-(3,4-dichlorophenyl)-*N′*,*N′*-dimethyl-

RN: 3134-12-1 **MP** (°C)**:** 119
MW: 337.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.745E-05	1.600E-02	22	M161	1 0 0 0 1	

3581. $C_{16}H_{14}Cl_2O_3$

Chlorobenzilate
Ethyl 4,4′-dichlorobenzilate
Acaraben
Benzilen
Folbex
Kopmite

RN: 510-15-6 **MP** (°C)**:** 36
MW: 325.19 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.998E-05	1.300E-02	20	F311	1 2 2 2 1	

3582. $C_{16}H_{14}Cl_2O_4$

Diclotop-methyl
Methyl (+/–)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate

RN: 51338-27-3 **MP** (°C)**:** 40
MW: 341.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.465E-04	5.000E-02	22	M161	1 0 0 0 1	

3583. $C_{16}H_{14}FNO$

6H-Dibenz[b,e]azepin-6-one, 5-(2-fluoroethyl)-5,11-dihydro-

RN: 155206-48-7 **MP** (°C)**:**
MW: 255.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.917E-04	7.448E-02	ns	M381	0 1 1 1 2	pH 7.0

3584. $C_{16}H_{14}N_2O$

Methaqualone
Quaalude
Mandrax
Somnafac

RN: 72-44-6 **MP** (°C)**:** 114–117
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-03	2.999E-01	23	P094	0 0 0 0 0	

3585. $C_{16}H_{14}N_2O_2$

C.I. Disperse blue 14
9,10-Anthracenedione, 1,4-bis(methylamino)-

RN: 2475-44-7 **MP** (°C)**:** 226
MW: 266.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-07	3.728E-05	25	B333	0 0 0 0 0	

3586. $C_{16}H_{14}N_2O_3$

3-(Hydroxymethyl)phenytoin
3-(Hydroxymethyl)-5,5-diphenyl-2,4-imidazolidinedione

RN: 21616-46-6 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.959E-04	1.400E-01	22	B154	1 1 1 1 1	0.1M HCl

3587. $C_{16}H_{14}N_2O_4$

C.I. Disperse blue 26
9,10-Anthracenedione, 1,5-dihydroxy-4,8-bis(methylamino)-
Resiren blue TG
Navilene blue GL
PTB 31

RN: 3860-63-7 **MP** (°C)**:** 217
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-08	2.028E-05	25	B333	0 0 0 0 0	

3588. $C_{16}H_{14}O_3$

Ketoprofen
2-(*meta*-Benzoylphenyl) propionic acid
Orudis
Alrheumat
Oruvail

RN: 22071-15-4 **MP** (°C)**:** 94
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.509E-04	6.380E-02	5	F306	1 0 1 2 2	intrinsic
9.045E-04	2.300E-01	21	B331	1 2 2 1 1	pH 7.4
3.696E-04	9.399E-02	22.5	B422	2 0 2 2 2	
4.640E-04	1.180E-01	25	A408	2 0 1 2 0	int
2.006E-04	5.100E-02	25	A427	0 0 0 0 0	
5.646E-04	1.436E-01	25	F306	1 0 1 2 2	intrinsic
1.156E-03	2.939E-01	32	C411	2 1 1 2 1	
8.066E-04	2.051E-01	37	F306	1 0 1 2 2	intrinsic
5.112E-04	1.300E-01	37	Y421	0 0 0 0 0	
3.933E-05	1.000E-02	amb	L434	0 0 0 0 0	
2.006E-04	5.100E-02	rt	H302	0 0 2 1 2	intrinsic
8.219E-04	2.090E-01	rt	R431	0 0 0 0 0	Average

3589. $C_{16}H_{14}O_3$

Fenbufen
3-(4-Biphenylylcarbonyl) propionic acid
Lederfen

RN: 36330-85-5 **MP** (°C)**:** 185
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-06	9.409E-04	5	F306	1 0 1 2 2	intrinsic
1.000E-05	2.543E-03	24.99	K447	0 0 0 0 0	pH 2.0
6.430E-05	1.635E-02	25	C314	0 0 0 0 0	
6.410E-05	1.630E-02	25	C314	0 0 0 0 0	
8.700E-06	2.212E-03	25	F301	1 1 0 0 1	pH 2.0, *sic*

(*continued*)

3589. $C_{16}H_{14}O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-06	2.212E-03	25	F306	1 0 1 2 2	intrinsic
1.800E-05	4.577E-03	37	F306	1 0 1 2 2	intrinsic
7.865E-06	2.000E-03	rt	H302	0 0 2 1 1	intrinsic

3590. $C_{16}H_{15}ClN_2$

Medazepam
7-Chloro-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepine
Nobrium
RN: 2898-12-6 **MP** (°C)**:**
MW: 270.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.083E-02	37	L011	1 0 2 1 1	

3591. $C_{16}H_{15}Cl_2NO_2$

Clomeprop
2-(2,4-Dichloro-3-methylphenoxy)-*N*-phenylpropanamide
RN: 84496-56-0 **MP** (°C)**:**
MW: 324.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-08	3.168E-05	ns	R427	0 0 0 0 0	

3592. $C_{16}H_{15}Cl_3OS_2$

2-(*p*-Methylthiophenyl)-2-(*p*-methylsulfinylphenyl)-1,1,1-trichloroethane
RN: 28463-05-0 **MP** (°C)**:** 133-136
MW: 393.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.174E-06	1.250E-03	ns	K117	0 1 2 1 1	

3593. $C_{16}H_{15}Cl_3O_2$

Methoxychlor
1,1′-(2,2,2-Trichloroethylidene)-bis[4-methoxybenzene]
Maralate
Methoxy DDT
Marlate
Chemform
RN: 72-43-5 **MP** (°C)**:** 82.5
MW: 345.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.786E-08	2.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.302E-07	4.500E-05	25	B083	2 2 1 2 1	particle size 5 µm

(*continued*)

3593. $C_{16}H_{15}Cl_3O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-07	5.000E-05	25	P085	0 0 0 0 0	
2.893E-07	1.000E-04	25	W025	1 0 2 2 2	
2.748E-07	9.500E-05	35	B083	2 2 1 2 1	particle size 5 µm
5.352E-07	1.850E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.794E-06	6.200E-04	ns	K117	0 1 2 1 1	
8.679E-09	3.000E-06	ns	K138	0 0 0 0 2	
2.314E-06	8.000E-04	ns	M110	0 0 0 0 0	EFG
1.794E-06	6.200E-04	ns	M138	0 1 0 0 1	
3.472E-07	1.200E-04	ns	M344	0 0 0 0 1	
2.089E-07	7.222E-05	ns	R427	0 0 0 0 0	

3594. $C_{16}H_{15}Cl_3O_2S_2$

2,2-bis(*p*-Methylsulfinylphenyl)-1,1,1-trichloroethane
2-(*p*-Methylsulfoxidephenyl)-1,1,1-trichloroethane
RN: 28396-87-4 **MP** (°C)**:** 150–153
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.077E-05	2.900E-02	ns	K117	0 1 2 1 1	

3595. $C_{16}H_{15}Cl_3O_4S_2$

2,2-bis(*p*-Methylsulfonylphenyl)-1,1,1-trichloroethane
RN: 30665-94-2 **MP** (°C)**:** 236.0
MW: 441.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.395E-06	1.500E-03	ns	K117	0 1 2 1 1	

3596. $C_{16}H_{15}Cl_3S_2$

2,2-*bis*-(*p*-Methylthiophenyl)-1,1,1-trichloroethane
RN: 19679-38-0 **MP** (°C)**:** 115-117
MW: 377.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E-06	5.700E-04	ns	K117	0 1 2 1 1	

3597. $C_{16}H_{15}FN_2O_5$

1-Butyryloxymethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Butyryloxymethyl-3-benzoyl-5-fluorouracil
RN: 97108-48-0 **MP** (°C)**:** 81–82
MW: 334.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.855E-04	6.200E-02	22	B321	0 0 0 0 0	pH 4.0

3598. $C_{16}H_{15}NO$

4-Cyano-4′-propyloxybiphenyl
3 COB
RN: 52709-86-1 **MP** (°C)**:**
MW: 237.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-07	2.136E-04	21	D300	2 2 1 1 2	

3599. $C_{16}H_{15}NO_2$

N-Butyl-1,8-naphthalimide
Naphthalimide, *N*-butyl-
1H-Benz[de]isoquinoline-1,3(2H)-dione, 2-butyl-
RN: 6914-62-1 **MP** (°C)**:** 95
MW: 253.30 **BP** (°C)**:** 412.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	5.066E-03	23	B410	2 1 2 2 2	

3600. $C_{16}H_{15}NO_2$

Cinnamyl anthranilate
2-Propen-1-ol, 3-phenyl-, 2-aminobenzoate
2-Aminobenzoic acid 3-phenyl-2-propenyl ester
3-Phenyl-2-propen-1-yl anthranilate
3-Phenyl-2-propenyl 2-aminobenzoate
Cinnamyl alcohol
RN: 87-29-6 **MP** (°C)**:** 60
MW: 253.30 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.080E-07	2.300E-04	ns	B338	0 0 0 0 1	

3601. $C_{16}H_{15}NO_3$

Benzoylphenylalanine
N-Benzoyl-DL-phenylalanine
RN: 2901-76-0 **MP** (°C)**:**
MW: 269.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.156E-03	8.500E-01	25.1	N026	0 0 0 0 0	

3602. $C_{16}H_{15}NO_4$
Benzoyltyrosine
N-Benzoyl-L-tyrosine
RN: 2566-23-6 **MP** (°C)**:**
MW: 285.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.680E+00	25.1	N026	0 0 0 0 0	

3603. $C_{16}H_{15}N_5$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-nitrile, 11-cyclopropyl-5,11-dihydro-4-methyl
RN: **MP** (°C)**:**
MW: 277.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-05	5.035E-03	ns	M381	0 1 1 1 2	pH 7.0

3604. $C_{16}H_{15}N_5O_4S$
2,5-Disulfanilamidopyridine
RN: **MP** (°C)**:**
MW: 373.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-03	4.950E-01	37	R058	1 2 1 1 2	

3605. $C_{16}H_{16}$
1,2,3,6,7,8-Hexahydropyrene
RN: 1732-13-4 **MP** (°C)**:** 133
MW: 208.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	2.291E-04	4	K049	1 0 2 1 1	

3606. $C_{16}H_{16}ClN_3O_3S$
Metolazone
2-Methyl-3-(*o*-tolyl)-6-sulfamyl-7-chloro-1,2,3,4-tetrahydro-4-quinazolinone
Zaroxolyn
Mykrox
Diulo
RN: 17560-51-9 **MP** (°C)**:** 256.0
MW: 365.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.321E-05	3.410E-02	10	B030	1 0 1 1 2	
1.339E-04	4.900E-02	20	B030	1 0 1 1 2	

(*continued*)

3606. $C_{16}H_{16}ClN_3O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-04	6.030E-02	25	B030	1 0 1 1 2	
1.971E-04	7.210E-02	30	B030	1 0 1 1 2	
2.236E-04	8.180E-02	35	B030	1 0 1 1 2	
2.733E-04	1.000E-01	36	B030	1 0 1 1 2	
1.640E-04	6.000E-02	37	H013	1 0 0 0 0	
2.952E-04	1.080E-01	40	B030	1 0 1 1 2	
3.799E-04	1.390E-01	45	B030	1 0 1 1 2	
4.155E-04	1.520E-01	50	B030	1 0 1 1 2	

3607. $C_{16}H_{16}N_2$

3,4,7,8-Tetramethyl-1,10-phenanthroline

RN: 1660-93-1 **MP** (°C)**:** 278.5
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-06	1.512E-03	25.04	B094	1 2 1 2 1	

3608. $C_{16}H_{16}N_2O_4$

Phenmedipham

Methyl *m*-hydroxycarbanilate *m*-methylcarbanilate

RN: 13684-63-4 **MP** (°C)**:** 143
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.33E-05	<1.00E-02	20	B200	1 0 0 0 0	
3.330E-06	1.000E-03	20	F311	1 2 2 2 1	
1.397E-05	4.194E-03	25	H434	0 0 0 0 0	
3.330E-05	1.000E-02	ns	M061	0 0 0 0 1	
9.989E-06	3.000E-03	rt	M161	0 0 0 0 0	

3609. $C_{16}H_{16}N_2O_4$

Desmedipham

Ethyl *m*-hydroxycarbanilate carbanilate

Carbamic acid, *N*-phenyl-, 3-((ethoxycarbonyl)amino)phenyl ester

Betanex

Betanal-475

Betamix 70 WP

RN: 13684-56-5 **MP** (°C)**:** 120
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-05	7.000E-03	rt	M161	0 0 0 0 0	
2.331E-05	7.000E-03	rt	R304	0 0 0 0 0	

3610. $C_{16}H_{16}N_4$
Disperse black 1
RN: 6054-48-4 **MP** (°C)**:**
MW: 264.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-07	7.930E-05	25	B333	0 0 0 0 0	

3611. $C_{16}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′3′-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-2,4-dimethyl-
RN: 135794-77-3 **MP** (°C)**:**
MW: 280.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.346E-05	1.499E-02	ns	M381	0 1 1 1 2	pH 7.0

3612. $C_{16}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-cyclobutyl-5,11-dihydro-5-methyl-
RN: 135794-88-6 **MP** (°C)**:**
MW: 280.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.911E-04	8.160E-02	ns	M381	0 1 1 1 2	pH 7.0

3613. $C_{16}H_{16}N_6O_4S$
2,5-Disulfanilamidopyrimidine
RN: **MP** (°C)**:**
MW: 388.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.664E-05	2.200E-02	37	R046	1 2 1 1 1	

3614. $C_{16}H_{16}O_2$
4-Methoxy-3,3′-dimethylbenzophenone
RN: 41295-28-7 **MP** (°C)**:** 62.25
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.323E-06	2.000E-03	20	M161	1 0 0 0 0	

3615. $C_{16}H_{16}O_3$

Ethyl benzoyl benzoate

RN: 106396-19-4 **MP** (°C)**:**
MW: 256.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.901E-04	9.999E-02	ns	F014	0 0 0 0 1	

3616. $C_{16}H_{16}O_3$

Anisyl phenylacetate
p-Methoxybenzyl phenylacetate
Phenylacetic acid, *p*-methoxybenzyl ester

RN: 102-17-0 **MP** (°C)**:**
MW: 256.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	5.126E-01	25	D407	1 0 2 2 2	
2.000E-03	5.126E-01	ns	S460	0 0 0 0 0	

3617. $C_{16}H_{17}ClN_2S$

Chlorphenethazine
2-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-ethanamide

RN: 2095-24-1 **MP** (°C)**:**
MW: 304.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-05	4.573E-03	ns	G023	0 0 1 1 1	

3618. $C_{16}H_{17}ClN_4O_3$

C.I. Disperse red 13
4-Nitro-2-chloro-4′-[ethyl(2-hydroxyethyl)amino]azobenzene
Acetoquinone light rubine BLZ
Acetamine rubine B
Acetate fast rubine B

RN: 3180-81-2 **MP** (°C)**:** 133
MW: 348.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-08	1.151E-05	25	B333	0 0 0 0 0	

3619. $C_{16}H_{17}ClN_4O_4$

C.I. Disperse red 7
Ethanol, 2,2′-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]*bis*-
RN: 4540-00-5 **MP** (°C)**:** 190
MW: 364.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.013E-04	25	B333	0 0 0 0 0	

3620. $C_{16}H_{17}NO$

Diphenamid
Dyamid
Enide
N,N-Dimethyl-α-phenylbenzeneacetamide
N,N-Dimethyldiphenylacetamide
Diherbid
RN: 957-51-7 **MP** (°C)**:** 132
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	2.399E-01	25	M061	1 0 0 0 1	
1.086E-03	2.600E-01	25	M161	1 0 0 0 2	
1.090E-03	2.609E-01	27	B200	1 0 0 0 2	
1.086E-03	2.600E-01	ns	B185	0 0 0 0 0	
2.079E-02	4.975E+00	ns	B200	0 0 0 0 0	
1.086E-03	2.600E-01	ns	H042	0 0 0 0 2	

3621. $C_{16}H_{17}NO_4$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-amino-2-oxoethyl ester, (*S*)
Naproxen, *N,N*-glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-amino-2-oxoethyl ester
Naproxen *N,N*-glycolamide ester
RN: 114665-17-7 **MP** (°C)**:** 139.5
MW: 287.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.183E-04	3.400E-02	21	B331	1 2 2 1 2	pH 7.4
1.183E-04	3.400E-02	21	B331	0 0 0 0 0	

3622. $C_{16}H_{17}N_3O_4S$
Cephalexin
Cefanex
C-Lexin
Keflex
Cefalexin
RN: 15686-71-2 **MP** (°C)**:**
MW: 347.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.724E-02	5.990E+00	10	O305	2 2 1 2 2	noncrystalline
1.569E-01	5.450E+01	15	O305	2 2 1 2 2	noncrystalline
1.416E-01	4.920E+01	20	O305	2 2 1 2 2	noncrystalline
3.598E-02	1.250E+01	25	P311	0 0 0 0 0	EFG
1.330E-02	4.620E+00	25	U001	0 0 0 0 0	
3.500E-03	1.216E+00	35	E311	0 0 0 0 0	

3623. $C_{16}H_{17}N_3O_4S.H_2O$
Cephalexin (monohydrate)
RN: 23325-78-2 **MP** (°C)**:**
MW: 365.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.694E-02	1.350E+01	25	M165	1 0 0 0 2	

3624. $C_{16}H_{17}N_5O_5$
Dis. A. 12
Ethanol, 2-[[4-[(2,4-dinitrophenyl)azo]phenyl]ethylamino]-
RN: 62570-20-1 **MP** (°C)**:**
MW: 359.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	7.187E-04	25	B333	0 0 0 0 0	

3625. $C_{16}H_{17}N_5O_6$
Dis. A. 14
4-[bis(2-Hydroxyethyl)amino]-2′,4′-dinitroazobenzene
RN: 60129-67-1 **MP** (°C)**:**
MW: 375.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	2.252E-03	25	B333	0 0 0 0 0	

3626. $C_{16}H_{18}ClNO_4S$

Oxathiin carboxanilide

Benzoic acid, 2-chlloro-5-[[(5,6-dihydro-2-methyl-1,4-oxathiin-3-yl)carnonyl]amino]isopropyl Ester

RN: 135812-04-3 **MP** (°C)**:** 130

MW: 355.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.653E-06	1.300E-03	25	O319	0 0 0 0 0	

3627. $C_{16}H_{18}FN_3O_3$

Norfloxacin

Noroxin

RN: 70458-96-7 **MP** (°C)**:**

MW: 319.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-04	2.700E-01	6	Y421	0 0 0 0 0	
6.576E-04	2.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
6.263E-04	2.000E-01	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer
2.505E-02	8.000E+00	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
5.950E-04	1.900E-01	25	A414	1 0 1 1 1	
1.159E-03	3.700E-01	25	Y421	0 0 0 0 0	
2.662E-03	8.500E-01	40	Y421	0 0 0 0 0	

3628. $C_{16}H_{18}NO_5P$

Diphenylmorpholidophosphate

RN: **MP** (°C)**:**

MW: 335.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.844E-03	2.295E+00	25	A040	1 0 0 0 2	

3629. $C_{16}H_{18}N_2O_3$

Difenoxuron

N-4-(4′-Methoxyphenoxy)phenyl-*N′*,*N′*-dimethylurea

C-3470

RN: 14214-32-5 **MP** (°C)**:** 138.5

MW: 286.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.985E-05	2.000E-02	20	M161	1 0 0 0 1	
6.985E-05	2.000E-02	ns	M061	0 0 0 0 1	

3630. $C_{16}H_{18}N_2O_4S$
Penicillin G
Benzylpenicillin
Pfizerpen
RN: 61-33-6 **MP** (°C)**:**
MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	2.675E+00	25	U001	0 0 0 0 0	

3631. $C_{16}H_{18}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-(1,1-dimethylethyl)-5,11-dihydro-5-methyl-
RN: 135794-80-8 **MP** (°C)**:**
MW: 282.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.416E-05	3.997E-03	ns	M381	0 1 1 1 2	pH 7.0

3632. $C_{16}H_{18}N_4O_2$
Dye III
4[[(4-Diethylamino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 298.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-07	2.715E-04	97.40	B198	1 2 1 1 1	

3633. $C_{16}H_{18}N_4O_2$
Dis. A. 5
4-Nitro-4′-diethylaminoazobenzene
4-Nitro-4′-*N,N*-diethylaminoazobenzene
DEANAB
RN: 3025-52-3 **MP** (°C)**:** 152
MW: 298.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-11	1.193E-08	25	B333	0 0 0 0 0	

3634. $C_{16}H_{18}N_4O_3$

Disperse red 1
Dye IV
C.I. Disperse red 1
1-[*N*-Ethyl-*N*-(2-hydroxyethyl)amino]-4-(4-nitrophenylazo)benzene
4-Nitro-4′-[ethyl(2-hydroxyethyl)amino]azobenzene
RN: 2872-52-8 **MP** (°C)**:** 161
MW: 314.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-07	1.697E-04	25	B333	0 0 0 0 0	
5.400E-06	1.697E-03	60	B198	1 2 1 1 1	
6.521E-06	2.050E-03	60	P313	0 0 0 0 0	average of 2
1.082E-05	3.400E-03	70	P313	0 0 0 0 0	average of 2
1.310E-05	4.118E-03	71.80	B198	1 2 1 1 2	
1.797E-05	5.650E-03	80	P313	0 0 0 0 0	average of 2
3.120E-05	9.808E-03	84.10	B198	1 2 1 1 2	
3.388E-05	1.065E-02	90	P313	0 0 0 0 0	average of 2
7.130E-05	2.241E-02	97.40	B198	1 2 1 1 2	

3635. $C_{16}H_{18}N_4O_4$

Disperse red 19
Dye V
C.I. Disperse red 19
2-[(2-Hydroxyethyl)[4-(4-nitrophenylazo)phenyl]amino]ethanol
4′-[(*N,N*-Dihydroxyethyl)amino]-4-nitroazobenzene
RN: 2734-52-3 **MP** (°C)**:** 209
MW: 330.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-07	2.345E-04	25	B333	0 0 0 0 0	
1.170E-05	3.865E-03	60	B198	1 2 1 1 2	
3.030E-05	1.001E-02	71.80	B198	1 2 1 1 2	
8.330E-05	2.752E-02	84.10	B198	1 2 1 1 2	
2.100E-04	6.937E-02	97.40	B198	1 2 1 1 2	

3636. $C_{16}H_{18}O_3$

Naproxen ethyl esterv
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, ethyl ester, (alpha*S*)-
RN: 31220-35-6 **MP** (°C)**:**
MW: 258.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.645E-06	1.200E-03	21	B331	1 2 2 1 2	pH 7.4
4.645E-06	1.200E-03	21	B331	0 0 0 0 0	

3637. $C_{16}H_{19}ClN_2$

Chlorpheniramine
1-(*p*-Chlorophenyl)-1-(2-pyridyl)-3-dimethylaminopropane
RN: 132-22-9 **MP** (°C)**:** <25
MW: 274.80 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.496E+00	37.5	L034	2 2 0 1 2	pH 7.4

3638. $C_{16}H_{19}NO_7$

Benzoic acid, 2-(acetyloxy)-, 2-[(2-ethoxy-2-oxoethyl)methylamino]-2-oxoethyl ester
RN: 116482-77-0 **MP** (°C)**:** 47.5
MW: 337.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-03	9.600E-01	21	N335	0 0 0 0 0	

3639. $C_{16}H_{19}N_3O_2$

C.I. Solvent yellow 58
p-[bis(2-Hydroxyethyl)amino]azobenzene
4-[bis(2-Hydroxyethyl)amino]azobenzene
RN: 2452-84-8 **MP** (°C)**:** 134
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.139E-02	25	B333	0 0 0 0 0	

3640. $C_{16}H_{19}N_3O_4S$

Cephradine
Anspor
Velosef
RN: 38821-53-3 **MP** (°C)**:** 140
MW: 349.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-02	2.130E+01	ns	F181	0 0 0 0 2	

3641. $C_{16}H_{19}N_3O_4S$

Ampicillin
(2*S*,5*R*,6*R*)-6-[(*R*)-2-Amino-2-phenylacetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0] heptane-2-carboxylic acid
Aminobenzylpenicillin
Unasyn
Wymox
Totacillin

RN: 69-53-4 **MP** (°C)**:**
MW: 349.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.293E-02	1.500E+01	7.5	P009	1 0 2 1 0	EFG
3.721E-02	1.300E+01	20	P009	1 0 2 1 0	EFG
2.890E-02	1.010E+01	21	M044	2 0 2 2 2	
3.978E-02	1.390E+01	25	H051	1 2 2 2 2	
6.600E-03	2.306E+00	25	K444	0 0 0 0 0	
3.434E-02	1.200E+01	30	P009	1 0 2 1 0	EFG
3.291E-02	1.150E+01	40	P009	1 0 2 1 0	EFG

3642. $C_{16}H_{19}N_3O_4S.3H_2O$

Ampicillin (trihydrate)

RN: 7177-48-2 **MP** (°C)**:** 198
MW: 403.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-02	5.700E+00	7.5	P009	1 0 2 1 0	EFG
1.487E-02	6.000E+00	20	P009	1 0 2 1 0	EFG
1.873E-02	7.558E+00	21	M044	2 0 2 2 2	
1.983E-02	8.000E+00	30	P009	1 0 2 1 0	EFG
2.479E-02	1.000E+01	40	P009	1 0 2 1 0	EFG

3643. $C_{16}H_{19}N_3O_5S$

Amoxicillin

RN: 61336-70-7 **MP** (°C)**:**
MW: 365.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	4.000E+00	ns	K444	0 0 0 0 0	

3644. $C_{16}H_{19}N_3O_5S.3H_2O$

Amoxicillin (trihydrate)
4-Thia-1-azabicyclo(3,2,0)heptane-2-carboxylic acid (trihydrate)
RN: 61336-70-7 **MP** (°C)**:**
MW: 419.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.54E-03	~4.00E+00	ns	B188	0 0 0 0 0	

3645. $C_{16}H_{19}N_5O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-dimethylamino)-11-ethyl-5,11-dihydro-4-methyl-
RN: 135795-08-3 **MP** (°C)**:**
MW: 297.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E-05	4.002E-03	ns	M381	0 1 1 1 2	pH 7.0

3646. $C_{16}H_{19}N_5O_2$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-[(2-hydroxyethyl) methylamino
RN: 155206-46-5 **MP** (°C)**:**
MW: 313.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	1.368E-01	ns	M381	0 1 1 1 2	pH 7.0

3647. $C_{16}H_{19}O_4P$

Butyl diphenyl phosphate
RN: 2752-95-6 **MP** (°C)**:**
MW: 306.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3648. $C_{16}H_{20}I_3N_3O_7$

1,3-Benzenedicarboxamide, *N*-(2-hydroxyethyl)-*N′*-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-
RN: 77868-44-1 **MP** (°C)**:**
MW: 747.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.625E-02	1.961E+01	25	P091	0 0 0 0 0	

3649. $C_{16}H_{20}I_3N_3O_7$

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N′*-(2-hydroxyethyl)-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(*RS*)

RN: 77868-43-0 **MP** (°C)**:**
MW: 747.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.374E-02	4.762E+01	25	P091	0 0 0 0 0	

3650. $C_{16}H_{20}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(hydroxyacetyl)amino]-2,4,6-triiodo- [*RS*-(*RS**,*RS**)]-

RN: 77868-40-7 **MP** (°C)**:**
MW: 763.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.317E-02	1.768E+01	25	P091	0 0 0 0 0	

3651. $C_{16}H_{20}I_3N_3O_8$

1,3-Benzenedicarboxamide, 5-[(hydroxyacetyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 77868-41-8 **MP** (°C)**:**
MW: 763.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.282E-02	4.031E+01	25	P091	0 0 0 0 0	

3652. $C_{16}H_{20}N_4O_2$

Apazone
APZ
Azapropazone

RN: 13539-59-8 **MP** (°C)**:** 247
MW: 300.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.472E-01	35	H091	1 2 2 2 1	*sic*
2.896E-04	8.700E-02	rt	H302	0 0 2 1 1	intrinsic

3653. $C_{16}H_{20}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-isobutylpyrimidine

RN: **MP** (°C)**:**
MW: 348.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.091E-05	3.800E-03	37	R076	1 2 0 0 1	

3654. $C_{16}H_{20}N_8O_2S$

6-[D-2-Amino-2-(4-aminophenyl)-acetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3,2,0]hept-2-yl-5-t

RN: **MP** (°C)**:**
MW: 388.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.277E-03	2.050E+00	25	B148	2 2 2 1 2	

3655. $C_{16}H_{20}O_6P_2S_3$

Temephos
O,O′-(Thiodi-4,1-phenylene)bis(*O,O′*-dimethylphosphorothioate)
Abate
Tetramethyl *O,O′*-thiodi-*p*-phenylene phosphorothioate
Abaphos
Tetrafenphos

RN: 3383-96-8 **MP** (°C)**:**
MW: 466.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-08	9.000E-06	10	B324	0 0 0 0 0	
1.929E-08	8.998E-06	10	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B300	2 1 1 1 2	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
1.501E-06	7.002E-04	30	B324	0 0 0 0 0	
1.501E-06	7.000E-04	30	B324	0 0 0 0 0	

3656. $C_{16}H_{21}ClN_3S$

Methylene blue
Methylenblau
C.I. 52015

RN: 61-73-4 **MP** (°C)**:**
MW: 322.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.02E-01	~3.30E+01	20	F300	1 0 0 0 0	

3657. $C_{16}H_{21}NO$

N,N-Heptamethylenecinnamamide
Octahydro-1-(1-oxo-3-phenyl-2-propenyl) azocine

RN: 59832-06-3 **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	6.230E-02	ns	H350	0 0 0 0 0	

3658. $C_{16}H_{21}NO$

N-Cycloheptylcinnamamide
N-Cycloheptyl-3-phenyl-2-propenamide
RN: 59831-98-0 **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-06	8.688E-04	ns	H350	0 0 0 0 0	

3659. $C_{16}H_{21}NO_2$

Propranolol
2-Propanol, 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-
RN: 525-66-6 **MP** (°C)**:**
MW: 259.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-04	3.100E-02	22.5	B422	0 0 0 0 0	
3.123E-04	8.099E-02	25	S450	0 0 0 0 0	
3.092E-08	8.020E-06	32	M458	0 0 0 0 0	

3660. $C_{16}H_{21}NO_2S$

m-Carboxyloctylphenylisothiocyanate
3-Carboxyloctylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 291.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.748E-02	25	K032	2 2 0 1 1	

3661. $C_{16}H_{21}NO_3$

Piperidine, 1-[(benzoyloxy)acetyl]-2-ethyl-
RN: 115178-69-3 **MP** (°C)**:** 54.5
MW: 275.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.889E-03	5.200E-01	22	N317	1 1 2 1 2	

3662. $C_{16}H_{21}NO_3$

Piperidine, 1-[(benzoyloxy)acetyl]-2,6-dimethyl-
RN: 115178-70-6 **MP** (°C)**:** 118
MW: 275.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.448E-04	1.500E-01	22	N317	1 1 2 1 2	

3663. $C_{16}H_{21}NO_3$

Acetamide, 2-(benzoyloxy)-*N*-cyclohexyl-*N*-methyl-

RN: 106231-65-6 **MP** (°C)**:**
MW: 275.35 **BP** (°C)**:** 439.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.084E-04	1.400E-01	22	B427	1 0 0 1 1	

3664. $C_{16}H_{21}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-(diethylamino)-1-methyl-2-oxoethyl ester

RN: 118247-09-9 **MP** (°C)**:** 40.5
MW: 307.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.499E-02	7.680E+00	21	N335	0 0 0 0 0	

3665. $C_{16}H_{21}N_3$

Tripelennamine
N-Benzyl-*N′*,*N′*-dimethyl-*N*-2-pyridylethylenediamine
PBZ
Pelamine

RN: 91-81-6 **MP** (°C)**:** <25
MW: 255.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	5.873E-01	30	L068	1 0 0 1 0	EFG
1.500E-02	3.830E+00	37.5	L034	2 2 0 1 2	pH 7.4

3666. $C_{16}H_{22}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *n*-octyl ester
2,4-Dichlorophenoxyacetic acid capryl ester

RN: 1928-44-5 **MP** (°C)**:**
MW: 333.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.128E-05	7.092E-03	ns	M120	0 0 1 1 2	

3667. $C_{16}H_{22}N_4O$

Neohetramine
N,N-Dimethyl-*N′*-(*p*-methoxybenzyl)-*N′*-(2-pyrimidyl)ethylenediamine
Tonzilamine
RN: 91-85-0 **MP** (°C)**:**
MW: 286.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	5.441E+00	37.5	L034	2 2 0 1 2	pH 7.4

3668. $C_{16}H_{22}N_4O_2S$

2-Sulfanilamido-4-methyl-5-*n*-amylpyrimidine
RN: 71119-35-2 **MP** (°C)**:** 188-190
MW: 334.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-05	2.800E-02	29	C049	0 0 0 0 0	

3669. $C_{16}H_{22}N_4O_6$

2′-Valeryl-6-methoxypurine arabinoside
2′-Trimethylacetyl-6-methoxypurine arabinoside
RN: 121032-22-2 **MP** (°C)**:** 118–120
MW: 366.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-01	8.793E+01	37	C348	0 0 0 0 0	pH 7.00
1.070E-01	3.920E+01	37	C348	0 0 0 0 0	pH 7.00

3670. $C_{16}H_{22}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-pivalate-β-D-arabinofuranosyl)]-9H-purine (hemihydrate)
RN: 121032-42-6 **MP** (°C)**:** glass
MW: 375.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-02	1.336E+01	37	M378	1 2 1 1 2	pH 7.2

3671. $C_{16}H_{22}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-valerate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 142963-77-7 **MP** (°C)**:** foam
MW: 375.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-03	6.457E-01	37	M378	1 2 1 1 2	pH 7.2

3672. $C_{16}H_{22}O_4$

Dibutyl phthalate
n-Butyl phthalate
RN: 84-74-2 **MP** (°C)**:** –35
MW: 278.35 **BP** (°C)**:** 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.455E-05	1.240E-02	10	S198	2 1 2 2 2	
3.952E-05	1.100E-02	15	H069	1 0 1 1 1	
3.630E-05	1.010E-02	20	L300	2 1 0 2 2	
3.880E-05	1.080E-02	20	S198	2 1 2 2 2	
3.593E-04	1.000E-01	22	N311	1 0 1 1 2	
3.377E-05	9.400E-03	22	Y419	0 0 0 0 0	
6.574E-05	1.830E-02	23.5	S171	2 1 2 2 2	
3.126E-05	8.700E-03	25	D336	0 0 0 0 0	
3.449E-05	9.600E-03	25	D336	0 0 0 0 0	
4.670E-05	1.300E-02	25	F067	1 0 2 2 2	
1.609E-02	4.480E+00	25	F070	1 0 0 0 2	*sic*
4.095E-05	1.140E-02	30	S198	2 1 2 2 2	
1.437E-03	4.000E-01	rt	M161	0 0 0 0 2	

3673. $C_{16}H_{22}O_4$

Diisobutyl phthalate
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) esterpalatinol
Phthalic acid diisobutyl ester
Palatinolic
RN: 84-69-5 **MP** (°C)**:**
MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.592E-04	9.999E-02	20	F070	1 0 0 0 2	
7.300E-05	2.032E-02	20	L300	2 1 0 2 2	
2.227E-05	6.200E-03	24	H116	2 1 0 0 2	
5.030E-06	1.400E-03	25	D336	0 0 0 0 0	

3674. $C_{16}H_{22}O_4$

tere-Butyl phthalate
RN: 30448-43-2 **MP** (°C)**:**
MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-06	1.100E-03	25	D336	0 0 0 0 0	

3675. $C_{16}H_{22}O_4$

Di-*n*-butyl *o*-phthalate

RN: **MP** (°C)**:** –35 C

MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.593E-05	1.000E-02	25	S417	0 0 0 0 0	

3676. $C_{16}H_{22}O_6$

Diethoxyethyl phthalate

bis(2-Ethoxyethyl) phthalate

RN: 605-54-9 **MP** (°C)**:**

MW: 310.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.271E-03	1.946E+00	ns	F014	0 0 0 0 2	

3677. $C_{16}H_{22}O_8.2H_2O$

Coniferin (dihydrate)

4-Hydroxy-3-methoxy-1-(γ-hydroxypropenyl)benzene-4-D-glucoside (dihydrate)

Abietin(dihydrate)

Coniferosi(dihydrate)

RN: 531-29-3 **MP** (°C)**:** 185

MW: 378.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-02	4.975E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3678. $C_{16}H_{22}O_{11}$

β-D-Glucose pentaacetate

β-Glucose-penta-acetat

RN: 604-69-3 **MP** (°C)**:** 131

MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.306E-03	9.000E-01	18	F300	1 0 0 0 0	

3679. $C_{16}H_{22}O_{11}$

α-D-Glucose pentaacetate
1,2,3,4,6-Penta-*O*-acetyl-α-D-glucose
Pentaacetate
Glucopyranose pentaacetate
Glucose pentaacetate;
α-D-Glucopyranose

RN: 604-68-2 **MP** (°C)**:** 109–111
MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	1.484E+00	ns	R427	0 0 0 0 0	

3680. $C_{16}H_{22}O_{11}$

α-Glucose pentaacetate
α-Glucose-penta-acetat

RN: 3891-59-6 **MP** (°C)**:** 110
MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.843E-03	1.500E+00	18	F300	1 0 0 0 1	

3681. $C_{16}H_{23}FN_2O_6$

1,3-bis(Pivaloyloxymethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1,3-bis(Pivaloyloxymethyl)-5-fluorouracil

RN: 66542-50-5 **MP** (°C)**:** 102–104
MW: 358.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.256E-04	4.500E-02	22	B321	0 0 0 0 0	pH 4.0

3682. $C_{16}H_{23}NO$

n-Heptylcinnamamide
2-Propenamide, *N*-heptyl-3-phenyl-

RN: 59831-99-1 **MP** (°C)**:**
MW: 245.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-06	1.865E-03	ns	H350	0 0 0 0 0	

3683. $C_{16}H_{23}NO_2$

Etoxadrol
(+)-2-(2-Ethyl-2-phenyl-1,3-dioxolan-4-yl)piperidine
RN: 28189-85-7 **MP** (°C)**:**
MW: 261.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-03	6.500E-01	20	K017	1 2 2 2 2	pH 10, intrinsic
1.098E-02	2.870E+00	30	K017	1 2 2 2 2	pH 10, intrinsic
4.668E-02	1.220E+01	40	K017	1 2 2 2 2	pH 10, intrinsic

3684. $C_{16}H_{23}NO_3$

Acetaminophen octanoate
Octanoic acid, 4-(acetylamino)phenyl ester
RN: 54942-41-5 **MP** (°C)**:** 103
MW: 277.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.605E-05	1.000E-02	25	B010	1 1 1 1 0	

3685. $C_{16}H_{23}NO_3S_2$

N-[2-(3,4-Dihydroxyphenyl)ethyl]-5-[(3*R*)-1,2-dithiolan-3-yl]-pentanamide
RN: **MP** (°C)**:**
MW: 341.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-06	3.600E-04	ns	S453	0 0 0 0 0	

3686. $C_{16}H_{23}NO_6$

Monocrotaline
(–)-Monocrotaline
RN: 315-22-0 **MP** (°C)**:** 202
MW: 325.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.644E-02	1.186E+01	ns	I312	0 0 0 0 0	

3687. $C_{16}H_{23}N_5O_5$

9-[5′-(*O*-Caproyl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-34-3 **MP** (°C)**:**
MW: 365.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-03	2.500E+00	ns	B134	0 1 1 1 1	

3688. $C_{16}H_{23}N_5O_5$
9-[5′-(*O-tert*-Butylacetyl)-β-D-arabinofuranosyl]adenine ester
RN: 68325-42-8 **MP** (°C)**:**
MW: 365.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.135E-02	7.800E+00	ns	B134	0 1 1 1 1	

3689. $C_{16}H_{24}N_2O_2$
N,N,N′,N′-Tetraethylterephthalamide
RN: 15394-30-6 **MP** (°C)**:**
MW: 276.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.528E+00	30	K019	1 0 0 0 1	

3690. $C_{16}H_{24}N_2O_2$
N,N,N′,N′-Tetraethylisophthalamide
RN: 13698-87-8 **MP** (°C)**:**
MW: 276.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	1.990E+02	30	K019	1 0 0 0 2	

3691. $C_{16}H_{24}N_4O_2$
2,5-Diaziridinyl-3,6-bis(propylamino)-1,4-benzoquinone
RN: 59886-47-4 **MP** (°C)**:** 140
MW: 304.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.29E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3692. $C_{16}H_{24}N_4O_6$
2,5-Diaziridinyl-3,6-bis(2′-hydroxyl-3′-hydroxylpropylamino)-1,4-benzoquinone
2,5-Diaziridinyl-3,6-bis(hydroxylethylmethylamino)-1,4-benzoquinone
RN: 59886-55-4 **MP** (°C)**:** 273
MW: 368.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.629E-01	6.000E+01	rt	C317	0 0 0 0 0	
8.143E-02	3.000E+01	rt	C317	0 0 0 0 0	

3693. $C_{16}H_{24}N_6$

1-(Methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine

RN: 125867-93-8 **MP** (°C)**:**

MW: 300.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-05	7.291E-03	25	B386	0 0 0 0 0	

3694. $C_{16}H_{24}O_3$

Nonyl *p*-hydroxybenzoate

Nonyl 4-hydroxybenzoate

RN: 38713-56-3 **MP** (°C)**:**

MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-03	1.275E+00	25	D081	1 2 2 1 2	

3695. $C_{16}H_{24}O_4$

3,4-Epoxy-6-methylcyclohexylmethyl-3,4-epoxy-6-methylcyclohexane carboxylate

EP 201

RN: 141-37-7 **MP** (°C)**:**

MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E-02	2.991E+00	ns	I313	0 0 0 0 0	

3696. $C_{16}H_{25}NOS$

S-Benzyl di-*sec*-butylthiocarbamate

Thiocarbazil

Tiocarbazil

RN: 36756-79-3 **MP** (°C)**:**

MW: 279.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.946E-06	2.500E-03	30	M161	1 0 0 0 1	

3697. $C_{16}H_{25}NO_2$
Butacarb
Carbamic acid, *N*-methyl-, 3,5-di-*tert*-butylphenyl ester
3,5-Di-*tert*-butylphenyl methylcarbamate
RN: 2655-19-8 **MP** (°C)**:** 102.9
MW: 263.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.695E-05	1.500E-02	20	M161	1 0 0 0 1	

3698. $C_{16}H_{25}NO_2$
Nonyl *p*-aminobenzoate
Nonyl 4-aminobenzoate
RN: 37139-21-2 **MP** (°C)**:**
MW: 263.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-06	2.687E-04	37	F006	1 1 2 2 2	

3699. $C_{16}H_{25}NO_3$
4-Propoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 15788-85-9 **MP** (°C)**:**
MW: 279.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.257E-01	ns	M066	0 0 0 0 1	

3700. $C_{16}H_{26}$
2-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-08	5.678E-06	25	S377	0 0 0 0 0	

3701. $C_{16}H_{26}$
3-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	8.299E-06	25	S377	0 0 0 0 0	

3702. $C_{16}H_{26}$
4-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-08	7.862E-06	25	S377	0 0 0 0 0	

3703. $C_{16}H_{26}$
5-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-08	7.643E-06	25	S377	0 0 0 0 0	

3704. $C_{16}H_{26}N_2O_2$
4-Propylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-54-3 **MP** (°C)**:**
MW: 278.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	2.867E-01	ns	M066	0 0 0 0 2	

3705. $C_{16}H_{26}O_2$
4-Octylphenol monoethoxylate
RN: 51437-89-9 **MP** (°C)**:**
MW: 250.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.195E-05	8.000E-03	20.5	A335	0 0 0 0 0	
3.200E-05	8.012E-03	20.5	A335	0 0 0 0 0	

3706. $C_{16}H_{26}O_5$
Artemether
RN: 71963-77-4 **MP** (°C)**:**
MW: 298.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		ns	K444	0 0 0 0 0	

3707. $C_{16}H_{26}O_6$

Triethylene glycol dibutyrate

RN: 26962-26-5 **MP** (°C)**:**
MW: 314.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.524E-02	7.937E+00	ns	F014	0 0 0 0 2	

3708. $C_{16}H_{28}N_3O_2$

Dioxyethylaminoazobenzene

RN: **MP** (°C)**:**
MW: 294.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.945E-04	8.670E-02	0	K036	1 0 0 0 2	
4.212E-04	1.240E-01	25	K036	1 0 0 0 2	
2.819E-03	8.300E-01	90	K036	1 0 0 0 2	

3709. $C_{16}H_{32}O_2$

Palmitic acid

Hexadecanoic acid

RN: 57-10-3 **MP** (°C)**:** 56
MW: 256.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.794E-05	4.600E-03	0	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20.0	R001	1 1 1 1 1	
3.200E-06	8.206E-04	25	J001	1 0 2 1 1	
1.200E-07	3.077E-05	25	R002	0 0 0 0 0	intrinsic
2.680E-06	6.872E-04	25	R002	0 0 0 0 0	
3.237E-05	8.300E-03	30	B136	1 0 2 1 1	
3.237E-05	8.300E-03	30.0	R001	1 1 1 1 1	
3.900E-05	1.000E-02	45	B136	1 0 2 1 1	
3.900E-05	1.000E-02	45.0	R001	1 1 1 1 1	
4.000E-06	1.026E-03	50	J001	1 0 2 1 1	
4.680E-05	1.200E-02	60	B136	1 0 2 1 1	
4.680E-05	1.200E-02	60.0	R001	1 1 1 1 1	
1.794E-05	4.600E-03	.0	R001	1 1 1 1 1	

3710. $C_{16}H_{34}$
2,2,4,4,6,8,8-Heptamethylnonane
RN: 4390-04-9 **MP** (°C)**:**
MW: 226.45 **BP** (°C)**:** 240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.369E-09	3.100E-07	25	T423	0 0 0 0 0	

3711. $C_{16}H_{34}$
3-Methylpentadecane
RN: 2882-96-4 **MP** (°C)**:** –22
MW: 226.45 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.328E-10	9.800E-08	23	C332	0 0 0 0 0	

3712. $C_{16}H_{34}$
Hexadecane
n-Hexadecane
Cetane
RN: 544-76-3 **MP** (°C)**:** 18.17
MW: 226.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-08	6.290E-06	25	F004	0 0 0 0 0	

3713. $C_{16}H_{34}$
2-Methylpentadecane
RN: 1560-93-6 **MP** (°C)**:** –7
MW: 226.45 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.681E-10	1.060E-07	23	C332	0 0 0 0 0	

3714. $C_{16}H_{34}O$
Hexadecanol
Cetyl alcohol
RN: 36653-82-4 **MP** (°C)**:** 49
MW: 242.45 **BP** (°C)**:** 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.699E-07	4.120E-05	22.5	G301	0 0 0 0 0	
1.700E-07	4.122E-05	25	R002	0 0 0 0 0	
3.300E-08	8.001E-06	34	K011	1 2 1 1 2	

(*continued*)

3714. $C_{16}H_{34}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.393E-08	1.550E-05	43	H030	2 2 2 2 2	
6.393E-08	1.550E-05	43	H103	1 2 2 2 2	
1.270E-07	3.079E-05	55	K011	1 2 1 1 2	
1.675E-07	4.060E-05	61	H030	2 2 2 2 2	
1.675E-07	4.060E-05	61	H103	1 2 2 2 2	

3715. $C_{16}H_{35}O_3P$

Dibutyl isooctyl phosphonate

RN: 108979-58-4 **MP** (°C)**:**
MW: 306.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3716. $C_{16}H_{35}O_4P$

Dibutyl octyl phosphate

RN: 25786-28-1 **MP** (°C)**:**
MW: 322.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.10E-04	<1.00E-01	25	B070	1 2 0 1 0	

3717. $C_{17}H_{11}NO_3$

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-phenyl-

RN: 74103-09-6 **MP** (°C)**:**
MW: 277.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-07	3.300E-05	25	P089	0 0 0 0 0	
1.388E-07	3.850E-05	37	P089	0 0 0 0 0	
1.677E-07	4.650E-05	51	P089	0 0 0 0 0	

3718. $C_{17}H_{12}$

1,2-Benzofluorene
Benzo[a]fluorene
11H-Benzo[a]fluorene

RN: 238-84-6 **MP** (°C)**:** 187
MW: 216.29 **BP** (°C)**:** 407

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-07	4.500E-05	25	M064	1 1 2 2 1	
2.100E-07	4.542E-05	25	M342	1 0 1 1 1	
2.081E-07	4.500E-05	ns	M344	0 0 0 0 2	

3719. $C_{17}H_{12}$

2,3-Benzofluorene
Benzo[b]fluorene
11H-Benzo[b]fluorene
RN: 243-17-4 **MP** (°C)**:** 209
MW: 216.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E-08	4.000E-06	25	B319	2 0 1 2 0	
9.247E-09	2.000E-06	25	M064	1 1 2 2 1	
9.250E-09	2.001E-06	25	M342	1 0 1 1 2	

3720. $C_{17}H_{12}ClFN_2O$

Nuarimol
Triminol
Trimidal
Gauntlet
2-Chloro-4′-fluoro-α-(5-pyrimidinyl)benzhydryl alcohol
α-(2-Chlorophenyl)-α-(4-fluorophenyl)-5-pyrimidinemethanol
RN: 63284-71-9 **MP** (°C)**:**
MW: 314.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	2.618E-02	ns	R427	0 0 0 0 0	

3721. $C_{17}H_{12}ClFN_3O_2$

α-(4-Chlorophenyl)-α-(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
X-7801
DuP 860
RN: **MP** (°C)**:**
MW: 344.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.612E-06	1.590E-03	22	M362	1 1 2 1 1	

3722. $C_{17}H_{12}ClNO_2S$

Fentiazac
4-(*p*-Chlorophenyl)-2-phenyl-5-thiazoleacetic acid
RN: 18046-21-4 **MP** (°C)**:** 161.1
MW: 329.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-06	3.100E-03	5	F306	1 0 1 2 2	intrinsic
9.600E-05	3.166E-02	25	C314	0 0 0 0 0	
9.612E-05	3.170E-02	25	C314	0 0 0 0 0	

(*continued*)

3722. $C_{17}H_{12}ClNO_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.080E-05	3.562E-03	25	F306	1 0 1 2 2	intrinsic
1.310E-05	4.320E-03	37	F306	1 0 1 2 2	intrinsic
1.072E-05	3.534E-03	ns	R427	0 0 0 0 0	

3723. $C_{17}H_{12}Cl_2N_2O$

Fenarimol
2,4′-Dichloro-α-(5-pyrimidinyl)benzhydryl alcohol
α-(2-Chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol
Tebulan
Rubigan 4AS
Rimidin

RN: 60168-88-9 **MP** (°C)**:** 118
MW: 331.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.136E-05	1.370E-02	25	M161	1 0 0 0 2	pH 7

3724. $C_{17}H_{12}Cl_2N_4$

Triazolam
8-Chloro-6-(*o*-chlorophenyl)-1-methyl-4H-*s*-triazolo[4,3-a][1,4]benzodiazepine
Apo-Triazo
Gen-Triazolam
Halcion
Novo-Triolam

RN: 28911-01-5 **MP** (°C)**:**
MW: 343.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.741E-05	3.000E-02	amb	L434	0 0 0 0 0	

3725. $C_{17}H_{12}Cl_{10}O_3$

Kelevan
Allied GC 9160
Despirol

RN: 4234-79-1 **MP** (°C)**:** 91
MW: 618.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.888E-06	5.500E-03	20	M164	1 0 0 0 1	

3726. $C_{17}H_{12}I_2O_3$
Benziodarone
Algocor
Amplivix
Dilafurane
RN: 68-90-6 **MP** (°C)**:**
MW: 518.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-05	5.881E-03	20	H301	0 0 0 0 0	

3727. $C_{17}H_{12}O_6$
Aflatoxin B1
AFB1
RN: 1162-65-8 **MP** (°C)**:** 268
MW: 312.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.803E-05	1.500E-02	ns	I306	0 0 0 0 0	

3728. $C_{17}H_{12}O_7$
Aflatoxin G1
RN: 1165-39-5 **MP** (°C)**:** 244
MW: 328.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.569E-05	1.500E-02	ns	I306	0 0 0 0 0	

3729. $C_{17}H_{13}ClN_4$
Alprazolam
8-Chloro-1-methyl-6-phenyl-4H-*s*-triazolo[4,3-a][1,4]benzodiazepine
Apo-Alpraz
Kalma
Novo-Alprazol
Nu-Alpraz
RN: 28981-97-7 **MP** (°C)**:**
MW: 308.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.267E-04	7.000E-02	amb	L434	0 0 0 0 0	
3.239E-04	1.000E-01	amb	L445	0 0 0 0 0	intrinsic

3730. $C_{17}H_{13}ClO_3$
Itanoxone
2′-Chloro-α-methylene-γ-oxo[1,1′-biphenyl]-4-butanoic acid
F 1379
RN: 58182-63-1 **MP** (°C)**:** 212
MW: 300.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.318E-04	1.900E-01	20	C112	2 0 1 1 2	

3731. $C_{17}H_{13}Cl_2N_3O_2$
α-(2,4-Difluorophenyl)-α-(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
A-9991
DuP 991
RN: **MP** (°C)**:**
MW: 362.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-05	7.000E-03	22	M362	1 1 2 1 1	

3732. $C_{17}H_{14}F_3N_3O_2S$
Celecoxib
4-[5-(4-Methylphenyl)-3-(trifluoromethyl)
Celebrex
SC-58635
YM-177
RN: 169590-42-5 **MP** (°C)**:**
MW: 381.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-05	7.000E-03	25	S415	0 0 0 0 0	
7.866E-06	3.000E-03	37	Y412	0 0 0 0 0	

3733. $C_{17}H_{14}N_2O$
1-*o*-Tolylazo-2-naphthol
Orange OT
Oil orange SS
1-(*o*-Tolylazo)-2-naphthol
RN: 2646-17-5 **MP** (°C)**:** 131
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-07	2.000E-04	30	R430	0 0 0 0 0	
1.000E-07	2.623E-05	rt	M163	0 0 0 0 1	

3734. $C_{17}H_{14}O_4S$

Rofecoxib
4-(4-Methylsulfonylphenyl)-3-phenyl-5H-furan-2-one
RN: 162011-90-7 **MP** (°C)**:**
MW: 314.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.605E-05	8.190E-03	24.99	D414	0 0 0 0 0	
2.863E-05	9.000E-03	25	S415	0 0 0 0 0	
2.977E-05	9.360E-03	29.99	D414	0 0 0 0 0	
3.556E-05	1.118E-02	34.99	D414	0 0 0 0 0	
2.545E-06	8.000E-04	37	Y421	0 0 0 0 0	

3735. $C_{17}H_{14}O_6$

Aflatoxin B2
RN: 7220-81-7 **MP** (°C)**:** 286
MW: 314.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-05	1.500E-02	ns	I306	0 0 0 0 0	

3736. $C_{17}H_{14}O_7$

Aflatoxin G2
RN: 7241-98-7 **MP** (°C)**:** 237
MW: 330.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.500E-02	ns	I306	0 0 0 0 0	

3737. $C_{17}H_{15}NO_3$

Cinnamyl acetaminophen
Cinnamic acid, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, cinnamate (ester)
RN: 20682-28-4 **MP** (°C)**:** 200–201
MW: 281.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.977E-06	1.400E-03	37	D029	0 0 0 0 0	

3738. $C_{17}H_{15}NO_5$

Benzoic acid, 2-(acetyloxy)-, 4-(acetylamino)phenyl ester

RN: 5003-48-5 **MP** (°C)**:** 174.5
MW: 313.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.383E-05	2.000E-02	21	N335	0 0 0 0 0	

3739. $C_{17}H_{16}Br_2O_3$

Bromopropylate
1-Methylethyl-4-bromo-α-(4-bromophenyl)-α-hydroxybenzeneacetate
Neoron
GS-19851
Phenisobromolate

RN: 18181-80-1 **MP** (°C)**:** 77
MW: 428.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.17E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.168E-05	5.000E-03	20	M161	1 0 0 0 0	

3740. $C_{17}H_{16}ClFN_2O_2$

Progabide
Butanamide, 4-[[(4-chlorophenyl)(5-fluoro-2-hydroxyphenyl)methylene]amino]-
Gabrene
SL 76-002

RN: 62666-20-0 **MP** (°C)**:**
MW: 334.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-04	3.716E-02	37	F309	1 0 2 2 2	
1.110E-04	3.716E-02	37	F318	2 2 0 0 2	

3741. $C_{17}H_{16}Cl_2O_3$

Chloropropylate
1-Methylethyl-4-chloro-α-(4-chlorophenyl)-α-hydroxybenzenacetate
Chlormite
Acaralate
G-24163
Rospin

RN: 5836-10-2 **MP** (°C)**:** 74
MW: 339.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.422E-06	1.500E-03	20	F311	1 2 2 2 1	
2.948E-05	1.000E-02	rt	M161	0 0 0 0 1	

3742. $C_{17}H_{16}N_2O_2S$
1-Sulfamethylnaphthalene
RN: **MP** (°C)**:**
MW: 312.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-05	1.000E-02	20	F073	1 2 2 2 1	

3743. $C_{17}H_{16}N_2O_3$
C.I. Disperse blue 3
1-[(2-Hydroxyethyl)amino]-4-(methylamino)-9,10-anthracenedione
C.I. 61505
RN: 2475-46-9 **MP** (°C)**:** 187
MW: 296.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.556E-05	25	B333	0 0 0 0 0	

3744. $C_{17}H_{16}N_2O_3S$
4-Sulfahydroxymethylnaphthalene
RN: **MP** (°C)**:**
MW: 328.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-04	5.500E-02	20	F073	1 2 2 2 1	

3745. $C_{17}H_{16}N_2O_4$
p-(*p*-Acetamidobenzamido)phenyl acetate
RN: 74973-19-6 **MP** (°C)**:**
MW: 312.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-05	1.218E-02	25	A066	1 0 1 1 1	

3746. $C_{17}H_{16}N_2O_4S$
1-Benzenesulfonyl-5-ethyl-5-phenyl-hydantoin
5-Ethyl-5phenyl-1(phenylsulfonyl)-2,4-imidazolidinedione
RN: 21413-25-2 **MP** (°C)**:**
MW: 344.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.782E-04	3.369E-01	37	F183	1 0 1 1 1	intrinsic

3747. $C_{17}H_{16}N_2O_5$

p-4-Acetaminophenyl acetaminophen
Acetamide, *N,N′*-[carbonylbis(oxy-4,1-phenylene)]*bis*-
Acetanilide, 4′-hydroxy-, carbonate (2:1) (ester)
RN: 19872-72-1 **MP** (°C)**:** 219.5–220
MW: 328.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-04	6.000E-02	37	D029	0 0 0 0 0	

3748. $C_{17}H_{17}ClO_6$

Griseofulvin
(2*S-trans*)-7-Chloro-2′,4,6-trimethoxy-6′-methylspiro[benzofuran-2(3H),1′-[2]cyclohexene]-3,4′-dione
Fulvicin
Grisactin
Grifulvin
Griseostatin
RN: 126-07-8 **MP** (°C)**:** 220.0
MW: 352.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-05	6.456E-03	15	E010	2 2 2 2 2	
2.466E-05	8.700E-03	20	N322	0 0 0 0 0	
3.260E-05	1.150E-02	21	E316	0 0 0 0 0	
3.175E-04	1.120E-01	21	M044	2 0 2 2 2	*sic*
4.025E-04	1.420E-01	21	M044	2 0 2 2 2	microsize, *sic*
2.126E-05	7.500E-03	22	C040	2 0 2 2 0	EFG
2.076E-05	7.325E-03	22	M382	2 1 1 1 1	average of 2
1.474E-05	5.200E-03	22.5	B422	2 0 2 2 2	
2.523E-05	8.900E-03	23	B362	0 0 0 0 0	
2.268E-05	8.000E-03	25	C037	2 1 2 2 2	
2.450E-05	8.643E-03	25	E010	2 2 2 2 2	
3.685E-05	1.300E-02	25	H015	1 0 0 0 1	
2.835E-05	1.000E-02	25	L033	1 0 2 1 1	
2.268E-05	8.000E-03	25	M457	0 0 0 0 0	
2.750E-05	9.700E-03	25	P096	0 0 0 0 0	
2.551E-05	9.000E-03	27	B043	1 0 1 2 0	EFG
2.835E-05	1.000E-02	30	M045	2 0 0 0 0	
4.000E-05	1.411E-02	30	O321	0 0 0 0 0	
4.252E-05	1.500E-02	30	O321	0 0 0 0 0	
3.510E-05	1.238E-02	35	E010	2 2 2 2 2	
3.969E-05	1.400E-02	37	B039	2 1 1 1 0	EFG
4.252E-05	1.500E-02	37	B043	1 0 1 2 0	EFG
3.969E-05	1.400E-02	37	B045	1 0 1 1 1	
4.054E-05	1.430E-02	37	F033	2 0 2 0 2	
3.968E-05	1.400E-02	37	G011	1 0 1 1 0	EFG
4.252E-05	1.500E-02	37	K018	1 0 0 0 1	
5.669E-05	2.000E-02	45	B043	1 0 1 2 0	EFG

(*continued*)

3748. $C_{17}H_{17}ClO_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.140E-05	2.166E-02	45	E010	2 2 2 2 2	
3.798E-05	1.340E-02	ns	D340	0 0 0 0 0	
2.835E-04	1.000E-01	ns	K444	0 0 0 0 0	
2.466E-05	8.700E-03	ns	N323	0 0 0 0 0	

3749. $C_{17}H_{17}Cl_2N$

Sertraline

(1*S*-*cis*)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-*N*-methyl-1-naphthalenamine

RN: 79617-96-2 **MP** (°C)**:**

MW: 306.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.27E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3750. $C_{17}H_{17}NO_2$

Apomorphine

Apomorphin

RN: 58-00-4 **MP** (°C)**:**

MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.069E-01	15	K059	2 2 2 0 0	
7.481E-02	2.000E+01	25	P312	0 0 0 0 0	

3751. $C_{17}H_{17}NO_5$

N-Benzyloxycarbonyl-L-tyrosine

Carbobenzoxytyrosine

RN: 1164-16-5 **MP** (°C)**:**

MW: 315.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.852E-03	1.530E+00	25.1	N026	0 0 0 0 0	

3752. $C_{17}H_{17}N_5O_5$

9-[5′-(*O*-Benzoyl)-β-D-arabinofuranosyl]adenine ester

RN: 42782-57-0 **MP** (°C)**:** 223.0

MW: 371.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E-04	8.000E-02	ns	B134	0 1 1 1 0	

3753. $C_{17}H_{18}ClNO_6$

Griseofulvin-4′-oxime

Spiro[benzofuran-2(3H),1′-[2]cyclohexene]-3,4′-dione, 7-chloro-2′,4,6-trimethoxy-6′-methyl-, 4′-oxime

RN: 13215-54-8 **MP** (°C)**:**
MW: 367.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.589E-04	1.320E-01	37	F033	2 0 2 0 2	

3754. $C_{17}H_{18}ClN_5O_6$

Dis. A. 8

Ethanol, 2,2′-[[4-[(2-chloro-4,6-dinitrophenyl)azo]-3-methylphenyl]imino]*bis*-

RN: 65125-87-3 **MP** (°C)**:**
MW: 423.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.119E-04	25	B333	0 0 0 0 0	

3755. $C_{17}H_{18}Cl_2N_4O_4$

Dis. A. 10

Ethanol, 2,2′-[4-(2,6-dichloro-4-nitrophenylazo)-*m*-tolylimino]di-

RN: 58528-60-2 **MP** (°C)**:**
MW: 413.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.546E-04	25	B333	0 0 0 0 0	

3756. $C_{17}H_{18}FN_3O_3$

Ciprofloxacin

1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic

Baycip

Velmonit

RN: 85721-33-1 **MP** (°C)**:**
MW: 331.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.117E-04	3.700E-02	6	Y421	0 0 0 0 0	
1.630E-04	5.400E-02	22.5	B422	2 0 2 2 2	
2.595E-04	8.600E-02	25	Y421	0 0 0 0 0	
4.225E-04	1.400E-01	30	Y421	0 0 0 0 0	
5.131E-04	1.700E-01	40	Y421	0 0 0 0 0	
3.730E+00	1.236E+03	c	B443	0 0 0 0 0	

3757. $C_{17}H_{18}N_2O_6$
Nifedipine
3,5-Pyridinedicarboxylicacid
RN: 21829-25-4 **MP** (°C)**:** 172–174
MW: 346.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-05	5.800E-03	25	B387	0 0 0 0 0	
2.887E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.738E-05	6.019E-03	ns	R427	0 0 0 0 0	

3758. $C_{17}H_{18}N_4O_3S$
4-Sulfanilamido-1-phenyl-2,3-dimethyl-5-pyrazolone
RN: 71119-16-9 **MP** (°C)**:**
MW: 358.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.352E-04	1.560E-01	37	R045	1 2 1 1 2	

3759. $C_{17}H_{19}ClN_2S$
4-Chloropromazine
4-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 13094-24-1 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-05	3.508E-03	ns	G023	0 0 1 1 1	

3760. $C_{17}H_{19}ClN_2S$
3-Chloropromazine
3-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 484-19-5 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.189E-03	ns	G023	0 0 1 1 1	

3761. $C_{17}H_{19}ClN_2S$
1-Chloropromazine
1-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 13100-13-5 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	3.826E-03	0	G023	0 0 0 0 1	

3762. $C_{17}H_{19}ClN_4O_4$

C.I. Disperse red 5

Ethanol, 2,2′-[[4-[(2-chloro-4-nitrophenyl)azo]-3-methylphenyl]imino]*bis*-

RN: 3769-57-1 **MP** (°C)**:** 192

MW: 378.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.440E-04	25	B333	0 0 0 0 0	

3763. $C_{17}H_{19}ClO_6$

Griseofulvin-4′-ol

Spiro[benzofuran-2(3H),1′-[2]cyclohexen]-3-one, 7-chloro-4′-hydroxy-2′,4,6-trimethoxy-6′-methyl-

RN: 13215-53-7 **MP** (°C)**:**

MW: 354.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E-04	2.529E-01	37	F033	2 0 2 0 2	average of 2

3764. $C_{17}H_{19}NO_3$

Piperine

Piperidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]-, (E,E)-

N-[(E,E)-Piperoyl]piperidine

RN: 94-62-2 **MP** (°C)**:** 130.0

MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	3.995E-02	15	K059	2 2 2 0 1	
1.402E-04	4.000E-02	18	F300	1 0 0 0 0	
3.504E-04	9.999E-02	rt	D021	0 0 1 1 0	

3765. $C_{17}H_{19}NO_3$

1-Methyl-1-nitro-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane

RN: 53982-07-3 **MP** (°C)**:**

MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.060E-06	2.300E-03	rt	C122	0 0 0 0 0	

3766. $C_{17}H_{19}NO_3$

Hydromorphone
Dilaudid
PMS-Hydromorphone
Dihydromorphinone

RN: 466-99-9 **MP** (°C)**:**
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.767E-03	1.931E+00	25	R338	0 0 0 0 0	

3767. $C_{17}H_{19}NO_3$

Morphine
Morphin
7,8-Didehydro-4,5-epoxy-17-methylmorphinan-3,6-diol

RN: 57-27-2 **MP** (°C)**:** 254dec
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.427E-01	15	K059	2 2 2 0 0	
5.222E-04	1.490E-01	20	B061	1 0 1 1 2	
5.257E-04	1.500E-01	20	F300	1 0 0 0 0	
1.209E-03	3.450E-01	25	R338	0 0 0 0 0	
7.200E-04	2.054E-01	30	L068	1 0 0 1 0	EFG
1.000E-03	2.853E-01	30	L069	1 0 1 1 0	EFG
8.761E-04	2.500E-01	35	R418	0 0 0 0 0	Intrinsic
1.051E-03	2.999E-01	rt	D021	0 0 1 1 0	

3768. $C_{17}H_{19}NO_3.H_2O$

Morphine (monohydrate)
Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl-(5α,6α)-, monohydrate

RN: 6009-81-0 **MP** (°C)**:** 254dec
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.328E-04	2.830E-01	c	D004	0 0 0 0 0	
3.064E-03	9.294E-01	h	D004	0 0 0 0 0	

3769. $C_{17}H_{19}NO_4$

1-Methyl-1-nitro-2,2-bis(*p*-methoxylphenyl)ethane

RN: 34197-26-7 **MP** (°C)**:**
MW: 301.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.854E-05	8.600E-03	rt	C122	0 0 0 0 0	

3770. $C_{17}H_{19}N_3$
Antazoline
Albalon-A
RN: 91-75-8 **MP** (°C)**:** 120
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	6.634E-01	30	L068	1 0 0 1 0	EFG
1.900E-02	5.042E+00	37.5	L034	2 2 0 1 2	pH 7.4

3771. $C_{17}H_{19}N_5O_6$
Dis. A. 1
Ethanol, 2,2′-[4-(2,4-dinitrophenylazo)-*m*-tolylimino]di-
Disperse violet 4K
Terasil violet P 4RT
RN: 41541-13-3 **MP** (°C)**:** 190
MW: 389.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-07	2.726E-04	25	B333	0 0 0 0 0	

3772. $C_{17}H_{20}ClN_5O_2$
1H-Purine-2,6-dione, 8-(2-amino-4-chlorophenyl)-3,7-dihydro-1,3-dipropyl-
1,3-Dipropyl-8-(2-amino-4-chlorophenyl)xanthine
PACPX
RN: 85872-51-1 **MP** (°C)**:**
MW: 361.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.76E-07	<1.00E-04	ns	H316	0 0 0 0 0	pH 7.4
1.105E-06	4.000E-04	ns	H316	0 0 0 0 0	0.1N HCL

3773. $C_{17}H_{20}N_2O$
Michler′s ketone
Tetramethyldiaminobenzophenone
bis[4-(Dimethylamino)phenyl]-methanone
p,p′-bis(*N,N*-Dimethylamino)benzophenone
4,4[-bis(Dimethylamino)benzophenone
RN: 90-94-8 **MP** (°C)**:** 172.0
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	3.998E-01	rt	D021	0 0 1 1 0	

3774. $C_{17}H_{20}N_2O_2$

Tropicamide

RN: 1508-75-4 **MP** (°C)**:**
MW: 284.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.032E-04	2.000E-01	25	C414	1 0 1 1 0	EFG

3775. $C_{17}H_{20}N_2S$

Promethazine
10-(2-Dimethylaminopropyl)phenothiazine
10-(2-Dimethylamino-2-methylethyl)phenothiazine
Fenergan
Protazine
Thiergan

RN: 60-87-7 **MP** (°C)**:** 60
MW: 284.43 **BP** (°C)**:** 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-06	3.839E-04	22.5	B440	0 0 0 0 0	
5.500E-05	1.564E-02	24	G023	2 0 1 1 1	
4.390E+00	1.249E+03	c	B443	0 0 0 0 0	

3776. $C_{17}H_{20}N_2S$

Promazine
Primazine
Sparine
Prozine

RN: 58-40-2 **MP** (°C)**:** 32
MW: 284.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.422E-02	24	G023	2 0 1 1 1	
5.000E-05	1.422E-02	ns	G023	0 0 0 0 1	

3777. $C_{17}H_{20}N_4O_4$

C.I. Disperse red 17
Ethanol, 2,2′-[[3-methyl-4-[(4-nitrophenyl)azo]phenyl]imino]*bis*-

RN: 3179-89-3 **MP** (°C)**:** 160
MW: 344.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	6.199E-04	25	B333	0 0 0 0 0	

3778. $C_{17}H_{20}N_4O_5$

Dis. A. 13
4-Nitro-2-methoxy-4′-di(β-hydroxyethyl)-aminoazobenzene
Ethanol, 2,2′-[[4-[(2-methoxy-4-nitrophenyl)azo]phenyl]imino]bis
Ethanol, 2,2′-[*p*-(2-methoxy-4-nitrophenylazo)phenylimino]di-
RN: 41541-14-4 **MP** (°C)**:**
MW: 360.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.207E-03	25	B333	0 0 0 0 0	
6.826E-04	2.460E-01	100	P313	0 0 0 0 0	

3779. $C_{17}H_{20}N_4O_5S$

Benzenesulfonic acid, 4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-
RN: 89073-57-4 **MP** (°C)**:**
MW: 392.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	1.300E+00	ns	H316	0 0 0 0 0	0.1N HCL
>6.12E-02	>2.40E+01	ns	H316	0 0 0 0 0	pH 7.4

3780. $C_{17}H_{20}N_4O_6$

Riboflavine
Riboflavin
Robiflavine
7,8-Dimethyl-10-ribitylisoalloxazine
Zinvit-G
E-101
RN: 83-88-5 **MP** (°C)**:** 290
MW: 376.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.657E-04	9.999E-02	20	A022	1 0 0 0 0	
2.250E-04	8.468E-02	25	A079	1 0 1 1 2	
2.657E-04	9.999E-02	25	D041	1 0 0 0 0	
1.754E-04	6.600E-02	25	D315	0 0 0 0 0	
2.192E-04	8.250E-02	30	C409	2 0 1 2 2	
3.959E-04	1.490E-01	37	E018	1 0 2 1 2	
2.089E-04	7.864E-02	ns	R427	0 0 0 0 0	

3781. $C_{17}H_{20}O_6$

Mycophenolic acid
6-(1,3-Dihydro-7-hydroxy-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic acid
RN: 24280-93-1 **MP** (°C)**:**
MW: 320.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.058E-05	1.300E-02	25	L333	1 1 1 1 0	

3782. $C_{17}H_{21}NO_2$

Napropamide
N,N-Diethyl-2-(1-naphthyloxy)propanamide
Devrinol 50W
Devrinol
Devrinol 10G
Devrinol 2E
RN: 15299-99-7 **MP** (°C)**:** 75.1
MW: 271.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	7.300E-02	20	M161	1 0 0 0 1	

3783. $C_{17}H_{21}NO_3$

Etodolac
(+/-)-1,8-Diethyl-1,3,4,9-tetrahydropyrano-(3,4-b)indole-1-acetic acid
Lodine
RN: 41340-25-4 **MP** (°C)**:**
MW: 287.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E-04	4.000E-02	37	Y421	0 0 0 0 0	

3784. $C_{17}H_{21}NO_4$

Scopolamine
Scopolamin
Hyoscine
Murocoll
Plexonal
Transderm-SCOP
RN: 51-34-3 **MP** (°C)**:** 59
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E-01	9.500E+01	15	F300	1 0 0 0 1	
3.296E-01	1.000E+02	ns	C109	0 0 0 0 1	

3785. $C_{17}H_{21}NO_4$
Cocaine
L-Cocaine
L-Cocain
RN: 50-36-2 **MP** (°C)**:** 98
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	1.213E+00	15	K059	2 2 2 0 0	
5.934E-03	1.800E+00	22	F300	1 0 0 0 1	
5.485E-03	1.664E+00	25	D004	0 0 0 0 0	
5.266E-03	1.597E+00	25	D041	1 0 0 0 1	
1.248E-02	3.786E+00	80	D041	1 0 0 0 1	

3786. $C_{17}H_{21}N_3O_2$
Dis. A. 2
Ethanol, 2,2′-[[3-methyl-4-(phenylazo)phenyl]imino]*bis*-
4-[bis(2-Hydroxyethyl)amino]-2-methylazobenzene
RN: 3771-38-8 **MP** (°C)**:** 111
MW: 299.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-05	2.275E-02	25	B333	0 0 0 0 0	

3787. $C_{17}H_{21}N_5O_2$
1H-Purine-2,6-dione, 8-(2-aminophenyl)-3,7-dihydro-1,3-dipropyl-
RN: 96445-34-0 **MP** (°C)**:** 276dec
MW: 327.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.05E-06	<1.00E-03	ns	H316	0 0 0 0 0	pH 7.4
1.222E-05	4.000E-03	ns	H316	0 0 0 0 0	0.1N HCL

3788. $C_{17}H_{21}N_5O_{10}$
9-(1,3-Dihemisuccinate-2-propoxymethyl)guanine
RN: 88110-76-3 **MP** (°C)**:** 167
MW: 455.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	4.730E+01	25	B360	0 0 0 0 0	

3789. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*RS**)]-

RN: 60166-94-1 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3790. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*RS**)]-

RN: 77942-93-9 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-01	1.150E+02	25	P091	0 0 0 0 0	

3791. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N′*-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-

RN: 77868-45-2 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3792. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*S*-(*S**,*S**)]-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3793. $C_{17}H_{22}I_3N_3O_8$

DL-Iopamidol

1,3-Benzenedicarboxamide, *N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-

L-Iopamidol

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*S**,*S**)]-

RN: 60166-93-0 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-01	4.737E+02	20	F178	1 0 0 0 1	EFG
1.580E-01	1.228E+02	20	F178	1 0 0 0 1	EFG
6.096E-01	4.737E+02	25	P091	0 0 0 0 0	
1.580E-01	1.228E+02	25	P091	0 0 0 0 0	
5.798E-01	4.505E+02	40	F178	1 0 0 0 1	EFG
1.963E-01	1.525E+02	40	F178	1 0 0 0 1	EFG
5.679E-01	4.413E+02	60	F178	1 0 0 0 1	EFG
3.120E-01	2.424E+02	60	F178	1 0 0 0 1	EFG
6.235E-01	4.845E+02	80	F178	1 0 0 0 1	EFG
5.209E-01	4.048E+02	80	F178	1 0 0 0 1	EFG
6.911E-01	5.370E+02	100	F178	1 0 0 0 1	EFG
7.098E-01	5.516E+02	100	F178	1 0 0 0 1	EFG

3794. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*S**)]-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3795. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*RS*)-

RN: 60208-45-9 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-01	1.379E+02	25	P091	0 0 0 0 0	

3796. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(*RS*,*S*)-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3797. $C_{17}H_{22}I_3N_3O_9$

1,3-Benzenedicarboxamide, 5-[(2,3-dihydroxy-1-oxopropyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 69698-47-1 **MP** (°C)**:**
MW: 793.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.573E-02	5.213E+01	25	P091	0 0 0 0 0	

3798. $C_{17}H_{22}I_3N_3O_9$

1,3-Benzenedicarboxamide, 5-[(2,3-dihydroxy-1-oxobutyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 129968-26-9 **MP** (°C)**:**
MW: 793.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.430E-02	4.306E+01	25	P091	0 0 0 0 0	

3799. $C_{17}H_{22}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-*n*-amylpyrimidine

RN: **MP** (°C)**:**
MW: 362.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.214E-05	4.400E-03	37	R076	1 2 0 0 1	

3800. $C_{17}H_{22}N_4O_7.0.75H_2O$

2′-(2-Methyl-3-one-pentanyl)-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-50-4 **MP** (°C)**:** 55–60
MW: 407.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.770E-02	3.577E+01	37	C348	0 0 0 0 0	pH 7.00

3801. $C_{17}H_{23}NO$
N,N-Octamethylenecinnamamide
Octahydro-1-(1-oxo-3-phenyl-2-propenyl)1H-azonine
RN: 59832-07-4 **MP** (°C)**:**
MW: 257.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	6.332E-02	ns	H350	0 0 0 0 0	

3802. $C_{17}H_{23}NO$
N-Cyclooctylcinnamamide
2-Propenamide, *N*-cyclooctyl-3-phenyl-
RN: 59832-00-7 **MP** (°C)**:**
MW: 257.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.660E-06	6.846E-04	ns	H350	0 0 0 0 0	

3803. $C_{17}H_{23}NO_3$
Hyoscyamine
Hyoscyamin
Benzeneacetic acid, α-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, [3(*S*)-*endo*]-
Daturine
Duboisine
L-Hyoscyamine
RN: 101-31-5 **MP** (°C)**:** 108.5
MW: 289.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.244E-02	3.600E+00	20	F300	1 0 0 0 2	
1.225E-02	3.546E+00	c	D004	0 0 0 0 0	

3804. $C_{17}H_{23}NO_3$
Atropine
Atropin
8-Methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropionate
Neo-diophen
Minims
RN: 51-55-8 **MP** (°C)**:** 115
MW: 289.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.592E+00	15	K059	2 2 2 0 1	
5.529E-03	1.600E+00	18	F300	1 0 0 0 1	

(*continued*)

3804. $C_{17}H_{23}NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E-03	1.996E+00	20	D041	1 0 0 0 0	
1.032E-02	2.987E+00	20	K052	1 1 1 1 2	
1.610E+00	4.659E+02	25	B443	0 0 0 0 0	
1.148E-02	3.322E+00	25	D004	0 0 0 0 0	
7.586E-03	2.195E+00	rt	D021	0 0 1 1 1	

3805. $C_{17}H_{23}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-[bis(1-methylethyl)amino]-2-oxoethyl ester

RN: 116482-76-9 **MP** (°C)**:** 108.9
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-04	1.800E-01	21	N335	0 0 0 0 0	

3806. $C_{17}H_{23}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-(dipropylamino)-2-oxoethyl ester

RN: 116482-75-8 **MP** (°C)**:** 50.5
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	7.200E-01	21	N335	0 0 0 0 0	

3807. $C_{17}H_{23}N_3O$

Aeo-antergan
1,2-Ethanediamine, *N*-[(4-methoxyphenyl)methyl]-*N′,N′*-dimethyl-*N*-2-pyridinyl-
Dorantamin
Anthisan
Dipane
Copsamine

RN: 91-84-9 **MP** (°C)**:**
MW: 285.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	3.425E+00	37.5	L034	2 2 0 1 2	pH 7.4

3808. $C_{17}H_{23}N_3O_2$
2-Methoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-methoxyquinoline-4-carboxamide
RN: 2716-98-5 **MP** (°C)**:**
MW: 301.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	9.042E-01	ns	B018	0 0 0 0 1	
3.000E-03	9.042E-01	ns	M066	0 0 0 0 0	

3809. $C_{17}H_{24}N_4O_5$
1,5-Dipivaloyloxymethyl allopurinol
RN: 98827-16-8 **MP** (°C)**:** 136–137
MW: 364.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.488E-05	2.000E-02	22	B322	0 0 0 0 0	
5.495E-05	2.003E-02	ns	R427	0 0 0 0 0	

3810. $C_{17}H_{24}N_4O_5$
2,5-Dipivaloyloxymethyl allopurinol
RN: 98827-17-9 **MP** (°C)**:** 145–146
MW: 364.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-04	4.500E-02	22	B322	0 0 0 0 0	

3811. $C_{17}H_{24}N_4O_6$
2′-Hexanyl-6-methoxypurine arabinoside
RN: 145913-39-9 **MP** (°C)**:**
MW: 380.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	7.190E+00	37	C348	0 0 0 0 0	pH 7.00

3812. $C_{17}H_{25}NO$
N-Octylcinnamamide
2-Propenamide, *N*-octyl-3-phenyl-
RN: 55030-48-3 **MP** (°C)**:**
MW: 259.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-06	3.606E-04	ns	H350	0 0 0 0 0	

3813. $C_{17}H_{25}NO_3$

Acetamide, 2-(benzoyloxy)-*N*,*N*-bis(2-methylpropyl)-

RN: 115193-33-4 **MP** (°C)**:** 44.5
MW: 291.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3814. $C_{17}H_{25}NO_3$

Acetamide, 2-(benzoyloxy)-*N*,*N*-acetamide, 2-(benzoyloxy)-*N*,*N*-dibutyl-

RN: 106231-57-6 **MP** (°C)**:** 25
MW: 291.39 **BP** (°C)**:** 428.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	B427	1 0 0 1 1	in 0.01M HCl
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3815. $C_{17}H_{25}NO_4$

Octyl acetaminophen
Carbonic acid, octyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, octyl carbonate (ester)

RN: 19872-70-9 **MP** (°C)**:** 82.5–83
MW: 307.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-05	4.400E-03	37	D029	0 0 0 0 0	

3816. $C_{17}H_{25}N_5O_6$

9-(1,3-Dibutyrate-2-propoxymethyl)guanine

RN: 88110-71-8 **MP** (°C)**:** 200
MW: 395.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-04	1.400E-01	25	B360	0 0 0 0 0	

3817. $C_{17}H_{26}ClNO_2$

Butachlor
N-(Butoxymethyl)-2-chloro-*N*-(2,6-diethylphenyl)acetamide
N-(Butoxymethyl)-2-chloro-2′,6′-diethylacetanilide
Machete
Butanex
Hiltachlor

RN: 23184-66-9 **MP** (°C)**:** <–5
MW: 311.86 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.413E-05	2.000E-02	20	M161	1 0 0 0 1	
6.412E-05	2.000E-02	ns	S460	0 0 0 0 0	
7.055E-05	2.200E-02	ns	Y414	0 0 0 0 0	
7.055E-02	2.200E+01	ns	Y414	0 0 0 0 0	

3818. $C_{17}H_{26}O_3$

Decyl-*p*-hydroxybenzoate
Decyl *p*-hydroxybenzoate
n-Decyl *p*-hydroxybenzoate

RN: 69679-30-7 **MP** (°C)**:** 58
MW: 278.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	8.909E-03	15	B355	0 0 0 0 0	
3.710E-05	1.033E-02	20	B355	0 0 0 0 0	
8.800E-05	2.450E-02	25	B355	0 0 0 0 0	
1.303E-03	3.629E-01	25	D081	1 2 2 1 2	*sic*
7.943E-05	2.211E-02	25	F322	2 0 1 1 0	EFG

3819. $C_{17}H_{27}NO_2$

Terbutol
2,6-Di-*tert*-butyl-*p*-tolyl methylcarbamate

RN: 1918-11-2 **MP** (°C)**:** 185
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E-05	6.500E-03	25	B200	1 0 0 0 0	
2.523E-05	7.000E-03	ns	H042	0 0 0 0 0	

3820. $C_{17}H_{27}NO_2$
Venlafaxine
RN: 93413-69-5 **MP** (°C)**:**
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.60E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3821. $C_{17}H_{27}NO_3$
Pramoxine
Pramocaine
RN: 140-65-8 **MP** (°C)**:**
MW: 293.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-05	3.574E-03	22.5	B440	0 0 0 0 0	

3822. $C_{17}H_{27}NO_3$
Stadacain
4-Butoxybenzoic acid 2-(diethyl-amino)ethyl ester
RN: 2350-32-5 **MP** (°C)**:** 146
MW: 293.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	3.814E-02	ns	M066	0 0 0 0 1	

3823. $C_{17}H_{27}NO_4$
Nadolol
Corgard
Nadolol
RN: 42200-33-9 **MP** (°C)**:**
MW: 309.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-02	8.300E+00	25	A412	1 0 2 2 1	int

3824. $C_{17}H_{28}$
4-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-09	2.092E-06	25	S377	0 0 0 0 0	

3825. $C_{17}H_{28}$
6-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	2.557E-06	25	S377	0 0 0 0 0	

3826. $C_{17}H_{28}$
3-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-08	2.789E-06	25	S377	0 0 0 0 0	

3827. $C_{17}H_{28}$
2-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-09	1.859E-06	25	S377	0 0 0 0 0	

3828. $C_{17}H_{28}$
5-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-08	2.324E-06	25	S377	0 0 0 0 0	

3829. $C_{17}H_{28}N_2O_2$
4-Butylaminobenzoic acid 2-(diethyl-amino)ethyl ester
RN: 3772-42-7 **MP** (°C)**:**
MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	1.199E-01	ns	M066	0 0 0 0 1	

3830. $C_{17}H_{28}N_2O_2$

Endomid

N,*N*,*N*′,*N*′-Tetraethyl-bicyclo(2.2.1)hept-5-ene-2,3-dicarboxamide

RN: 4582-18-7 **MP** (°C)**:**

MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.916E-02	1.730E+01	20	K050	1 1 1 1 2	

3831. $C_{17}H_{28}O_2$

4-Nonylphenol monoethoxylate

Ethanol, 2-(4-nonylphenoxy)-

RN: 104-35-8 **MP** (°C)**:**

MW: 264.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.048E-05	2.770E-03	2	A335	0 0 0 0 0	
1.050E-05	2.776E-03	2	A335	0 0 0 0 0	
1.063E-05	2.810E-03	10	A335	0 0 0 0 0	
1.060E-05	2.803E-03	10	A335	0 0 0 0 0	
1.074E-05	2.840E-03	14	A335	0 0 0 0 0	
1.080E-05	2.856E-03	14	A335	0 0 0 0 0	
1.140E-05	3.014E-03	20.5	A335	0 0 0 0 0	
1.142E-05	3.020E-03	20.5	A335	0 0 0 0 0	
1.280E-05	3.384E-03	25	A335	0 0 0 0 0	
1.275E-05	3.370E-03	25	A335	0 0 0 0 0	

3832. $C_{17}H_{34}O_2$

Margaric acid

Heptadecanoic acid

RN: 506-12-7 **MP** (°C)**:**

MW: 270.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-05	2.800E-03	0	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20.0	R001	1 1 1 1 1	
1.997E-05	5.400E-03	30	B136	1 0 2 1 1	
2.034E-05	5.500E-03	30.0	R001	1 1 1 1 1	
2.551E-05	6.900E-03	45	B136	1 0 2 1 1	
2.551E-05	6.900E-03	45.0	R001	1 1 1 1 1	
2.995E-05	8.100E-03	60	B136	1 0 2 1 1	
2.995E-05	8.100E-03	60.0	R001	1 1 1 1 1	
1.035E-05	2.800E-03	.0	R001	1 1 1 1 1	

3833. $C_{17}H_{36}N_2Ge$
Spirogermanium
2-[3-(Dimethylamino)propyl]-8,8-diethyl-2-aza-8-germaspiro[4.5]decane
RN: 41992-23-8 **MP** (°C)**:**
MW: 341.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-05	8.400E-03	22	M456	0 0 0 0 0	pH 12.5

3834. $C_{17}H_{36}O$
Heptadecanol
1-Heptadecanol
RN: 1454-85-9 **MP** (°C)**:** 58
MW: 256.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<=1E-7	<=2.56E-5	25	R002	0 0 0 0 0	

3835. $C_{18}H_{10}Cl_4$
2,4,4″,6-Tetrachloro-*p*-terphenyl
2,4,4″,6-Tetrachloro-1,1′:4′,1″-terphenyl
RN: 61576-97-4 **MP** (°C)**:**
MW: 368.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.606E-10	5.910E-08	4	D351	1 2 1 1 2	
4.728E-10	1.740E-07	25	D351	1 2 1 1 2	
1.106E-09	4.069E-07	40	D351	1 2 1 1 2	

3836. $C_{18}H_{10}I_6N_2O_7$
Ioglycamic acid
N,*N*′-bis(3-Carboxy-2,4,6-triiodophenyl)-diglycolamide
BE 419
RN: 2618-25-9 **MP** (°C)**:**
MW: 1127.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.773E-04	2.000E-01	ns	H055	0 0 0 0 0	

3837. $C_{18}H_{10}N_2O_2S$
Disperse brightener
2,2′-(2,5-Thiophenediyl)bisbenzoxazole
Unitex OB
Uvitex EBF
RN: 2866-43-5 **MP** (°C)**:** 219
MW: 318.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-08	9.551E-06	25	B333	0 0 0 0 0	

3838. $C_{18}H_{11}Cl_3$
2,4″,5-Trichloro-*p*-terphenyl
2,4″,5-Trichloro-1,1′:4′,1″-terphenyl
RN: 61576-93-0 **MP** (°C)**:**
MW: 333.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-10	1.010E-07	4	D351	1 2 1 1 2	
1.233E-09	4.115E-07	25	D351	1 2 1 1 2	
2.567E-09	8.564E-07	39	D351	1 2 1 1 2	

3839. $C_{18}H_{11}NO_3$
Samaron yellow
Supra light yellow GGL(IG)
RN: 1326-08-5 **MP** (°C)**:**
MW: 289.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-06	1.157E-03	98.59	M180	0 0 2 2 0	EFG
8.000E-06	2.314E-03	111.46	M180	0 0 2 2 0	EFG
1.000E-05	2.893E-03	112.94	M180	0 0 2 2 0	EFG
1.100E-05	3.182E-03	119.00	M180	0 0 2 2 0	EFG
1.300E-05	3.761E-03	125.25	M180	0 0 2 2 0	EFG
1.400E-05	4.050E-03	128.45	M180	0 0 2 2 0	EFG
2.200E-05	6.364E-03	152.37	M180	0 0 2 2 0	EFG

3840. $C_{18}H_{11}NO_3$
Disperse yellow 54
C.I. Disperse yellow 54
RN: 7576-65-0 **MP** (°C)**:**
MW: 289.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.893E-05	25	B333	0 0 0 0 0	
2.400E-07	6.943E-05	60.0	D093	1 2 1 2 0	EFG

(*continued*)

3840. $C_{18}H_{11}NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-07	1.880E-04	71.8	D093	1 2 1 2 0	EFG
1.600E-06	4.629E-04	84.1	D093	1 2 1 2 0	EFG
4.000E-06	1.157E-03	97.4	D093	1 2 1 2 0	EFG

3841. $C_{18}H_{12}$

Tetracene
Naphthacene
2,3-Benzanthracene

RN: 92-24-0 **MP** (°C)**:** 341
MW: 228.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-08	3.607E-06	20	E009	1 0 0 1 2	
6.600E-09	1.507E-06	25	K001	2 2 2 2 1	
2.497E-09	5.700E-07	25	M064	1 1 2 2 1	
2.500E-09	5.707E-07	25	M342	1 0 1 1 1	
4.380E-09	1.000E-06	27	D003	1 0 0 1 1	
2.497E-09	5.700E-07	ns	M344	0 0 0 0 2	
2.754E-09	6.288E-07	ns	R424	0 0 0 0 0	

3842. $C_{18}H_{12}$

Triphenylene
9,10-Benzphenanthrene
Isochrysene

RN: 217-59-4 **MP** (°C)**:** 199
MW: 228.30 **BP** (°C)**:** 425

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-08	2.694E-06	8	M082	1 1 1 2 2	
1.180E-08	2.694E-06	8	M151	2 1 2 2 2	
1.311E-08	2.992E-06	8.04	M183	1 2 1 1 2	
1.330E-08	3.036E-06	12.00	M082	1 1 1 2 2	
1.330E-08	3.036E-06	12.00	M151	2 1 2 2 2	
1.328E-08	3.033E-06	12.04	M183	1 2 1 1 2	
1.490E-08	3.402E-06	14.80	M082	1 1 1 2 2	
1.490E-08	3.402E-06	14.80	M151	2 1 2 2 2	
2.500E-07	5.707E-05	20	E009	1 0 0 1 1	
2.140E-08	4.886E-06	20.50	M082	1 1 1 2 2	
2.140E-08	4.886E-06	20.50	M151	2 1 2 2 2	
2.144E-08	4.894E-06	20.54	M183	1 2 1 1 2	
1.800E-07	4.109E-05	25	A325	2 1 2 2 1	
1.880E-07	4.292E-05	25	K001	1 0 2 1 2	
1.884E-07	4.300E-05	25	M064	1 1 2 2 1	
2.891E-08	6.600E-06	25.00	M151	2 1 1 2 1	
1.665E-07	3.800E-05	27	D003	1 0 0 1 1	
3.350E-08	7.648E-06	27.30	M082	1 1 1 2 2	

(*continued*)

3842. $C_{18}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.350E-08	7.648E-06	27.30	M151	2 1 2 2 2	
3.354E-08	7.657E-06	27.34	M183	1 2 1 1 2	
3.550E-08	8.105E-06	28.20	M082	1 1 1 2 2	
3.550E-08	8.105E-06	28.20	M151	2 1 2 2 2	
3.556E-08	8.117E-06	28.24	M183	1 2 1 1 2	
1.486E-08	3.393E-06	114.84	M183	1 2 1 1 2	
1.884E-07	4.300E-05	ns	M344	0 0 0 0 2	

3843. $C_{18}H_{12}$

1,2-Benzanthracene
Benzanthracene
1,2-Benzoanthracene

RN: 56-55-3 **MP** (°C)**:** 155
MW: 228.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-08	2.991E-06	6.90	M082	1 1 1 2 2	
1.310E-08	2.991E-06	6.90	M151	2 1 2 2 2	
1.311E-08	2.992E-06	6.94	M183	1 2 1 1 2	
1.660E-08	3.790E-06	10.70	M082	1 1 1 2 2	
1.660E-08	3.790E-06	10.70	M151	2 1 2 2 2	
1.657E-08	3.783E-06	11.14	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.24	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.30	M082	1 1 1 2 2	
2.100E-08	4.794E-06	14.30	M151	2 1 2 2 2	
1.583E-08	3.613E-06	14.34	M183	1 2 1 1 2	
2.365E-08	5.400E-06	15	B385	0 0 0 0 0	
2.446E-08	5.584E-06	18.14	M183	1 2 1 1 2	
2.770E-08	6.324E-06	19.30	M082	1 1 1 2 2	
2.770E-08	6.324E-06	19.30	M151	2 1 2 2 2	
2.775E-08	6.335E-06	19.34	M183	1 2 1 1 2	
3.670E-08	8.378E-06	23.10	M082	1 1 1 2 2	
3.670E-08	8.378E-06	23.10	M151	2 1 2 2 2	
3.669E-08	8.377E-06	23.14	M183	1 2 1 1 2	
3.507E-08	8.007E-06	23.64	M183	1 2 1 1 2	
1.927E-07	4.400E-05	24	H116	2 1 0 0 1	
4.117E-08	9.400E-06	25	B319	2 0 1 2 1	
4.056E-08	9.260E-06	25	B385	0 0 0 0 0	
5.694E-08	1.300E-05	25	D406	1 2 2 2 2	
4.310E-08	9.840E-06	25	K001	2 2 2 2 2	
3.900E-09	8.904E-07	25	K123	1 0 2 2 1	*sic*
2.497E-08	5.700E-06	25	L332	1 1 1 1 2	
6.132E-08	1.400E-05	25	M064	1 1 2 2 1	
4.117E-08	9.400E-06	25	M071	2 2 2 2 2	
6.130E-08	1.399E-05	25	M342	1 0 1 1 2	
4.117E-08	9.400E-06	25.00	M151	2 1 1 2 1	
3.774E-08	8.617E-06	25.04	M183	1 2 1 1 2	
4.818E-08	1.100E-05	27	D003	1 0 0 1 1	

(*continued*)

3843. $C_{18}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.344E-08	1.220E-05	29	M071	2 2 2 2 2	
5.344E-08	1.220E-05	29.00	M151	2 1 1 2 2	
5.436E-08	1.241E-05	29.54	M183	1 2 1 1 2	
5.580E-08	1.274E-05	29.70	M082	1 1 1 2 2	
5.580E-08	1.274E-05	29.70	M151	2 1 2 2 2	
5.567E-08	1.271E-05	29.74	M183	1 2 1 1 2	
7.635E-08	1.743E-05	35	B385	0 0 0 0 0	
6.132E-08	1.400E-05	ns	M344	0 0 0 0 2	

3844. $C_{18}H_{12}$

Chrysene

1,2-Benzphenanthrene

RN: 218-01-9 **MP** (°C)**:** 254

MW: 228.30 **BP** (°C)**:** 448

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-09	7.077E-07	6.50	M082	1 1 1 2 2	
3.100E-09	7.077E-07	6.50	M151	2 1 2 2 2	
3.500E-09	7.990E-07	11.00	M082	1 1 1 2 2	
3.500E-09	7.990E-07	11.00	M151	2 1 2 2 2	
6.130E-09	1.399E-06	20.40	M082	1 1 1 2 2	
6.130E-09	1.399E-06	20.40	M151	2 1 2 2 2	
6.139E-09	1.401E-06	20.44	M183	1 2 1 1 2	
9.199E-09	2.100E-06	23	P339	0 0 0 0 0	
7.446E-08	1.700E-05	24	H116	2 1 0 0 1	
7.360E-09	1.680E-06	24.00	M082	1 1 1 2 2	
7.360E-09	1.680E-06	24.00	M151	2 1 2 2 2	
7.367E-09	1.682E-06	24.04	M183	1 2 1 1 2	
4.818E-09	1.100E-06	25	B319	2 0 1 2 1	average of 2
6.570E-09	1.500E-06	25	D406	1 2 2 2 2	
2.760E-08	6.301E-06	25	K001	2 2 2 2 2	
2.628E-08	6.000E-06	25	L332	1 1 1 1 2	
8.761E-09	2.000E-06	25	M064	1 1 2 2 1	
7.884E-09	1.800E-06	25	M071	2 2 2 2 2	
8.760E-09	2.000E-06	25	M342	1 0 1 1 2	
7.884E-09	1.800E-06	25.00	M151	2 1 1 2 1	
8.280E-09	1.890E-06	25.30	M082	1 1 1 2 2	
8.280E-09	1.890E-06	25.30	M151	2 1 2 2 2	
8.283E-09	1.891E-06	25.34	M183	1 2 1 1 2	
6.570E-09	1.500E-06	27	D003	1 0 0 1 1	
9.680E-09	2.210E-06	28.70	M082	1 1 1 2 2	
9.680E-09	2.210E-06	28.70	M151	2 1 2 2 2	
9.689E-09	2.212E-06	28.74	M183	1 2 1 1 2	
9.637E-09	2.200E-06	29	M071	2 2 2 2 2	
9.637E-09	2.200E-06	29.00	M151	2 1 1 2 1	
8.761E-09	2.000E-06	ns	M344	0 0 0 0 2	
8.710E-09	1.988E-06	ns	R424	0 0 0 0 0	
3.400E-06	7.762E-04	ns	W005	0 0 1 2 1	*sic*

3845. $C_{18}H_{12}N_2$

2,2′-Biquinoline
2,2′-Biquinolyl
RN: 119-91-5 **MP** (°C)**:** 193
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-06	1.020E-03	24	H106	1 0 2 2 2	
3.980E-06	1.020E-03	24	M303	1 0 1 1 2	

3846. $C_{18}H_{12}N_4O$

4-Hydroxy-6,7-diphenylpteridine
4-Hydroxy-6:7-diphenylpteridine
RN: 102943-71-5 **MP** (°C)**:**
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-04	2.000E-01	20	A019	2 2 1 1 2	

3847. $C_{18}H_{13}ClFN_3$

Midazolam
8-Chloro-6-(*o*-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine
RN: 59467-70-8 **MP** (°C)**:**
MW: 325.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-04	5.400E-02	24	A404	2 0 2 2 2	intrinsic pH = 9.5

3848. $C_{18}H_{13}ClF_3NO_7$

Fluoroglycofen-ethyl
Super Blazer
Fluoroglycofen ethyl ester
Ethoxycarbonylmethyl-5-(2-chloro-4-trifluoromethylphenoxy)-2-nitrobenzoate-hyphen-ethoxy-2-oxoethyl 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoate
5-[2-Chloro-4-(trifluoromethyl)-phenoxy]-2-nitro-benzoic acid 2-ethoxy-2-oxoethyl ester
RN: 77501-90-7 **MP** (°C)**:**
MW: 447.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.349E-06	6.040E-04	ns	R427	0 0 0 0 0	

3849. $C_{18}H_{13}N$
6-Aminochrysene
6-Chrysenamine
RN: 2642-98-0 **MP** (°C)**:** 210
MW: 243.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-07	1.550E-04	24	H106	1 0 2 2 2	
6.370E-10	1.550E-07	ns	M349	0 2 1 1 2	

3850. $C_{18}H_{13}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-6-methyl-1-phenyl-
RN: 74103-08-5 **MP** (°C)**:**
MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.463E-08	1.300E-05	25	P089	0 0 0 0 0	
1.270E-07	3.700E-05	37	P089	0 0 0 0 0	
2.163E-07	6.300E-05	51	P089	0 0 0 0 0	

3851. $C_{18}H_{13}NO_3$
N-1-Naphthylphthalamic acid
Naptalam
2-((1-Naphthylamino)carbonyl)benzoic acid
Naphthylphthalamic acid
ALANAP-1
NPA
RN: 132-66-1 **MP** (°C)**:** 185
MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-04	2.000E-01	25	B200	1 0 0 0 2	
6.866E-04	2.000E-01	ns	B185	0 0 0 0 0	
6.866E-04	2.000E-01	ns	N013	0 0 0 0 2	
6.866E-04	2.000E-01	rt	M161	0 0 0 0 2	

3852. $C_{18}H_{14}$
o-Terphenyl
1,2-Diphenyl benzene
RN: 84-15-1 **MP** (°C)**:** 58
MW: 230.31 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-06	1.239E-03	25	A325	2 1 2 2 2	

3853. $C_{18}H_{14}$
m-Terphenyl
1,3-Diphenyl benzene
RN: 92-06-8 **MP** (°C)**:** 89
MW: 230.31 **BP** (°C)**:** 365

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.560E-06	1.511E-03	25	A325	2 1 2 2 2	

3854. $C_{18}H_{14}$
p-Terphenyl
1,4-Diphenyl benzene
RN: 92-94-4 **MP** (°C)**:** 213
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-08	1.796E-05	25	A325	2 1 2 2 1	

3855. $C_{18}H_{14}Cl_4N_2O$
Miconazole
1-[2-(2,4-Dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1H-imidazole
1-[2,4-Dichloro-β-[(2,4-dichlorobenzyl)oxy]phenethyl]imidazole
Conoderm
RN: 22916-47-8 **MP** (°C)**:**
MW: 416.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.80E-09	<2.00E-06	25	P348	0 0 0 0 0	
2.163E-04	9.000E-02	amb	L434	0 0 0 0 0	

3856. $C_{18}H_{14}N_4O$
Disperse yellow 23
Phenol, 4-[[4-(phenylazo)phenyl]azo]-
p-Hydroxy-*p*-bis(azobenzene)
RN: 6250-23-3 **MP** (°C)**:**
MW: 302.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-10	6.047E-08	25	B333	0 0 0 0 0	
1.300E-07	3.930E-05	71.8	D093	1 2 1 2 0	EFG
5.500E-07	1.663E-04	84.1	D093	1 2 1 2 0	EFG
2.300E-06	6.954E-04	97.4	D093	1 2 1 2 0	EFG

3857. $C_{18}H_{14}N_4O_2$
Disperse orange 1
Dye VI
C.I. Disperse orange 1
4-(*p*-Nitrophenylazo)diphenylamine
4-Anilino-4′-nitroazobenzene
4-(4-Nitrophenylazo)diphenylamine
RN: 2581-69-3 **MP** (°C)**:** 157
MW: 318.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-09	4.775E-07	25	B333	0 0 0 0 0	
3.000E-07	9.550E-05	84.10	B198	1 2 1 1 0	
1.420E-06	4.520E-04	97.40	B198	1 2 1 1 2	
4.900E-06	1.560E-03	111.60	B198	1 2 1 1 1	
1.950E-05	6.208E-03	127	B198	1 2 1 1 2	

3858. $C_{18}H_{14}N_4O_5S$
Sulfasalazine
Salicylazosulfapyridine
SASP
Sulcolon
Salazosulfapyridine
Salicylazosulfapyridine
RN: 599-79-1 **MP** (°C)**:** 240–245
MW: 398.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.510E-05	1.000E-02	ns	K444	0 0 0 0 0	

3859. $C_{18}H_{15}Cl_3N_2O$
Econazole
1-[2-[(4-Chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]-1H-imidazole
RN: 27220-47-9 **MP** (°C)**:**
MW: 381.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-04	3.700E-01	amb	L434	0 0 0 0 0	

3860. $C_{18}H_{15}Cl_4N_3O_4$
Miconazole nitrate-β cyclidextrin complexant
RN: 22832-87-7 **MP** (°C)**:**
MW: 479.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-04	1.773E-01	25	P348	0 0 0 0 0	

3861. $C_{18}H_{15}NO_3$
Oxaprozin
4,5-Diphenyl-2-oxazolepropanoic acid
4,5-Diphenyl-2-oxazole-propionic acid
Choledyl
Daypro
Oxaprozin
RN: 21256-18-8 **MP** (°C)**:**
MW: 293.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.364E-05	4.000E-03	37	Y421	0 0 0 0 0	

3862. $C_{18}H_{15}N_3O_5$
1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, methyl ester
RN: 104663-14-1 **MP** (°C)**:** 156.5
MW: 353.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-05	7.000E-03	21	N337	0 0 0 0 0	pH 5
1.900E-05	6.713E-03	21	N337	0 0 0 0 0	pH 5

3863. $C_{18}H_{15}O_4P$
Triphenyl phosphate
Phosphoric acid triphenyl ester
Triphenyl phosphoric acid ester
Phenyl phosphate
TPP
RN: 115-86-6 **MP** (°C)**:** 49
MW: 326.29 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.237E-06	7.300E-04	24	H116	2 1 0 0 2	
6.129E-05	2.000E-02	ns	F014	0 0 0 0 0	

3864. $C_{18}H_{16}ClNO_5$
Fenoxaprop-*p*-ethyl
Fenoxaprop-*p* ethyl ester
Propanoic acid
2-{4-{(6-Chloro-2-benzoxazolyl)oxy}phenoxy}-ethyl ester
RN: 71283-80-2 **MP** (°C)**:**
MW: 361.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-06	7.054E-04	ns	R427	0 0 0 0 0	

3865. $C_{18}H_{16}Cl_3N_3O_4$
Econazole nitrate
Pevaryl
Spectazole
R 14827
RN: 68797-31-9 **MP** (°C)**:**
MW: 444.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	7.115E-01	25	P348	0 0 0 0 0	

3866. $C_{18}H_{16}N_2O_3$
Benzoyltryptophan
N-Benzoyl-DL-tryptophan
RN: 2901-79-3 **MP** (°C)**:**
MW: 308.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-03	5.600E-01	25.1	N026	0 0 0 0 0	

3867. $C_{18}H_{16}N_4O_3S$
2-(*N*4-Acetylsulfanilylamino)-4-phenylpyrimidine
RN: **MP** (°C)**:**
MW: 368.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	3.600E-03	37	R076	1 2 0 0 1	

3868. $C_{18}H_{17}ClN_4O_6.0.5H_2O$
9-[5-*O*-(4-Chlorobenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 121032-34-6 **MP** (°C)**:** 122–124
MW: 429.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-04	8.081E-02	37	M378	1 2 1 1 2	pH 7.2

3869. $C_{18}H_{17}Cl_2NO_3$
Benzoylprop-ethyl
Ethyl *N*-benzoyl-*N*-(3,4-dichlorophenyl)-2-aminopropionate
FX 2182
N-Benzoyl-*N*-(3,4-dichlorophenyl)-DL-alanine ethyl ester
Enaven
Suffix
RN: 22212-55-1 **MP** (°C)**:** 70.5
MW: 366.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.461E-05	2.000E-02	25	M161	1 0 0 0 1	

3870. $C_{18}H_{17}N_5O_8$
6-Methoxy-9-(5-*O*-[4-nitrobenzoyl]-β-D-arabinofuranosyl)-9H-purine
RN: 121032-21-1 **MP** (°C)**:** 202–203
MW: 431.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.467E-02	37	M378	1 2 1 1 2	pH 7.2

3871. $C_{18}H_{18}ClNO_4$
Clanobutin
Butanoic acid, 4-[(4-chlorobenzoyl)(4-methoxyphenyl)amino]-
Bykahepar
RN: 30544-61-7 **MP** (°C)**:**
MW: 347.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.270E-04	4.417E-02	37	K093	1 2 1 1 2	pH 3.0

3872. $C_{18}H_{18}ClNO_5$
Etofibrate
3-Pyridinecarboxylic acid, 2-[2-(4-chlorophenoxy)-2-methyl-1-oxopropoxy]ethyl ester
Tricerol
Lipo-Merz
RN: 31637-97-5 **MP** (°C)**:**
MW: 363.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.276E-03	rt	G093	0 1 1 1 2	pH4

3873. $C_{18}H_{18}ClNO_5$

Benzoximate

RN: 29104-30-1 **MP** (°C)**:** 73
MW: 363.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	3.026E-02	ns	R427	0 0 0 0 0	

3874. $C_{18}H_{18}ClNS$

Chlorprothixene
Taractan
1-Propanamine, 3-(2-chloro-9H-thioxanthen-9-ylidene)-*N*,*N*-dimethyl-, (3Z)-
Rentovet

RN: 113-59-7 **MP** (°C)**:**
MW: 315.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.936E-05	1.243E-02	20	H301	0 0 0 0 0	
1.221E-06	3.858E-04	22.5	B440	0 0 0 0 0	

3875. $C_{18}H_{18}N_2O_4$

C.I. Disperse blue 23
1,4-bis[(2-Hydroxyethyl)amino]anthraquinone
Acetoquinone blue BF

RN: 4471-41-4 **MP** (°C)**:** 248
MW: 326.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-06	7.833E-04	25	B333	0 0 0 0 0	

3876. $C_{18}H_{18}N_4O_6$

9-[5-*O*-(Benzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 121032-31-3 **MP** (°C)**:** 202–204
MW: 386.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-05	2.859E-02	37	M378	1 2 1 1 2	pH 7.2

3877. $C_{18}H_{18}N_4O_6.0.75H_2O$

2′-Benzoyl-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-44-6 **MP** (°C)**:** 84–86
MW: 399.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-02	7.118E+00	37	C348	0 0 0 0 0	pH 7.00

3878. $C_{18}H_{18}N_8O_6$

7,7′-Succinylditheophylline

RN: 58447-18-0 **MP** (°C)**:**
MW: 442.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-03	7.211E-01	25	L067	1 0 1 1 2	

3879. $C_{18}H_{18}O_2$

Dienestrol
3,4-bis(4-Hydroxyphenyl)-2,4-hexadiene
Dehydrostilbestrol

RN: 84-17-3 **MP** (°C)**:** 227.5
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-05	3.000E-03	37	B039	2 1 1 1 0	EFG
1.122E-05	2.988E-03	ns	R427	0 0 0 0 0	

3880. $C_{18}H_{18}O_2$

Equilenin
3-Hydroxy-17-keto-δ(1,3,5-10,6,8)estrapentaene
1,3,5-10,6,8-Estrapentaen-3-ol-17-one

RN: 517-09-9 **MP** (°C)**:** 258
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	1.520E-03	25	L033	1 0 2 1 2	

3881. $C_{18}H_{18}O_3$

Flurecol-butyl
Flurenol-*n*-butyl ester
n-Butyl-9-hydroxyfluorene-(9)-carboxylate
RN: 2314-09-2 **MP** (°C)**:** 70
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.293E-02	3.650E+00	20	B200	1 0 0 0 2	*sic*
1.293E-04	3.650E-02	20	M161	1 0 0 0 2	*sic*

3882. $C_{18}H_{19}Cl_2NO_4$

Felodipine
3,5-Pyridinedicarboxylic acid, 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-, ethyl methyl ester
Plendil
RN: 72509-76-3 **MP** (°C)**:**
MW: 384.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.301E-06	5.000E-04	20	N322	0 0 0 0 0	
1.179E-05	4.530E-03	22	M382	2 1 1 1 1	

3883. $C_{18}H_{19}F_3N_2S$

4-Trifluoromethyl-*N*,*N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 3852-94-6 **MP** (°C)**:**
MW: 352.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.467E-03	ns	G023	0 0 1 1 0	

3884. $C_{18}H_{19}F_3N_2S$

Fluopromazine
Triflupromazine
RN: 146-54-3 **MP** (°C)**:** <25
MW: 352.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.762E-03	24	G022	2 0 1 1 1	
5.000E-06	1.762E-03	ns	F027	0 0 0 0 0	

3885. $C_{18}H_{19}NO$
Desmethyldoxepin
1-Propanamine, 3-dibenz[b,e]oxepin-11(6H)-ylidene-*N*-methyl-
RN: 1225-56-5 **MP** (°C)**:**
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-04	1.048E-01	25	E051	1 0 2 1 2	

3886. $C_{18}H_{19}N_2O_4$
N-Benzoyl-L-tyrosinamide acetate
RN: **MP** (°C)**:**
MW: 327.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	4.256E-02	25	A066	1 0 1 1 1	

3887. $C_{18}H_{19}N_3O_6S$
Cephaloglycin
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
RN: 3577-01-3 **MP** (°C)**:**
MW: 405.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	1.050E+01	25	P311	0 0 0 0 0	EFG

3888. $C_{18}H_{19}N_5O_3$
C.I. Disperse dye
Propanenitrile, 3-[(2-hydroxyethyl)[3-methyl-4-[(4-nitrophenyl)azo]phenyl]amino]-
Celliton discharge scarlet RNL
Celliton fast scarlet RN
RN: 6054-58-6 **MP** (°C)**:** 156
MW: 353.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-07	6.714E-05	25	B333	0 0 0 0 0	

3889. $C_{18}H_{19}N_5O_6.0.3H_2O$
9-[5-*O*-(4-Aminobenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.3 hydrate)
RN: 121032-39-1 **MP** (°C)**:** 198–200
MW: 406.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.383E-02	37	M378	1 2 1 1 2	pH 7.2

3890. $C_{18}H_{19}N_5O_6$
2′-(*o*-Aminobenzoyl)-6-methoxypurine arabinoside
RN: 121032-55-1 **MP** (°C)**:**
MW: 401.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.060E-02	8.268E+00	37	C348	0 0 0 0 0	pH 7.00

3891. $C_{18}H_{20}$
2,4-Diphenyl-4-methyl-2-pentene
RN: 6362-80-7 **MP** (°C)**:**
MW: 236.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-07	2.475E-05	ns	D001	0 0 0 0 2	

3892. $C_{18}H_{20}Cl_2O_2$
1-Dichloro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 7388-32-1 **MP** (°C)**:**
MW: 339.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.664E-08	2.600E-05	rt	C122	0 0 0 0 0	

3893. $C_{18}H_{20}N_4O_7S$
2′-(*p*-Methylbenzenesulfonyl)-6-methoxypurine arabinoside
RN: 145913-49-1 **MP** (°C)**:** 214–215
MW: 436.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-04	5.412E-02	37	C348	0 0 0 0 0	pH 7.00

3894. $C_{18}H_{20}O_2$
Equilin
3-Hydroxy-17-keto-δ(1,3,5-10,7)estratetraene
1,3,5(10),7-Estratetraen-3-ol-17-one
RN: 474-86-2 **MP** (°C)**:** 238
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.217E-06	1.400E-03	25	H049	0 0 0 0 0	
5.254E-06	1.410E-03	25	L033	1 0 2 1 2	

3895. $C_{18}H_{20}O_2$
Diethylstilbestrol
Diethylstilboestrol
Destrol
4,4′-(1,2-Diethyl-1,2-ethenediyl)bisphenol
Tylosterone
Vagestrol
RN: 56-53-1 **MP** (°C)**:** 169
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-05	1.200E-02	25	G009	1 0 1 1 1	
9.316E-05	2.500E-02	30	M007	2 2 1 2 2	average of 6
		amb	L434	0 0 0 0 0	

3896. $C_{18}H_{21}ClN_2$
Chlorocyclizine
Chlorcyclizine
RN: 82-93-9 **MP** (°C)**:**
MW: 300.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	3.008E-01	37.5	L034	2 2 0 1 2	pH 7.4

3897. $C_{18}H_{21}ClN_2S$
2-Chloro-*N*,*N*-dimethyl-10H-phenothiazine-10-butanamine
RN: 13094-23-0 **MP** (°C)**:**
MW: 332.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.664E-03	ns	G023	0 0 1 1 0	

3898. $C_{18}H_{21}ClO$
1-Chloro-1-methyl-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane
RN: 56265-27-1 **MP** (°C)**:**
MW: 288.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.540E-06	1.600E-03	rt	C122	0 0 0 0 0	

3899. $C_{18}H_{21}NO_3$
Codeine
Codein
Methylmorphin
7,8-Didehydro-4,5-α-epoxy-3-methoxy-17-methylmorphinan-6-α-ol
Nucofed
Robitussin AC
RN: 76-57-3 **MP** (°C)**:** 155
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-02	9.000E+00	20	A073	1 1 1 1 0	
2.672E-02	8.000E+00	20	F300	1 0 0 0 0	
2.760E-02	8.264E+00	20	K052	1 1 1 1 2	
1.591E-01	4.762E+01	25	E041	2 2 2 2 0	EFG, form III, recrystallized
3.242E-02	9.705E+00	25	E041	2 2 2 2 0	EFG, form II, recrystallized
3.176E-02	9.509E+00	25	E041	2 2 2 2 0	EFG, form I, recrystallized
3.571E-02	1.069E+01	25	R338	0 0 0 0 0	
3.340E-02	1.000E+01	30	A073	1 1 1 1 1	
3.674E-02	1.100E+01	40	A073	1 1 1 1 1	
4.342E-02	1.300E+01	50	A073	1 1 1 1 1	
5.010E-02	1.500E+01	60	A073	1 1 1 1 1	
6.013E-02	1.800E+01	70	A073	1 1 1 1 1	
6.347E-02	1.900E+01	80	A073	1 1 1 1 1	
5.578E-02	1.670E+01	80	F300	1 0 0 0 2	
8.017E-02	2.400E+01	90	A073	1 1 1 1 1	
1.069E-01	3.200E+01	100	A073	1 1 1 1 1	

3900. $C_{18}H_{21}NO_3$
Thebainone A
Morphinan-6-one, 7,8-didehydro-4-hydroxy-3-methoxy-17-methyl-
Thebainon
RN: 467-98-1 **MP** (°C)**:** 146
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.000E+00	20	F300	1 0 0 0 0	
2.839E-02	8.500E+00	100	F300	1 0 0 0 1	

3901. $C_{18}H_{21}NO_3.H_2O$
Codeine (monohydrate)
Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, monohydrate, (5α,6α)
RN: 6059-47-8 **MP** (°C)**:** 155
MW: 317.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.604E-02	8.264E+00	c	D004	0 0 0 0 0	

3902. $C_{18}H_{21}NO_4$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(dimethylamino)-2-oxoethyl ester, (*S*)
Naproxen, *N*,*N*-dimethyl glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(dimethylamino)-2-oxoethyl ester
Naproxen *N*,*N*-dimethyl glycolamide ester
RN: 114665-18-8 **MP** (°C)**:** 150.5
MW: 315.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.268E-05	4.000E-03	21	B331	1 2 2 1 2	pH 7.4
1.268E-05	4.000E-03	21	B331	0 0 0 0 0	

3903. $C_{18}H_{22}ClNO_4$
Oxycodone hydrochloride
4,5-Epoxy-14-hydroxy-3-methoxy-17-methylmorphinan-6-one hydrochloride
Endocet
Percocet
Supeudol
Roxicet
RN: 124-90-3 **MP** (°C)**:** 270–271
MW: 351.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.060E-01	1.429E+02	ns	S469	0 0 0 0 0	

3904. $C_{18}H_{22}N_2$
1-(Diphenylmethyl)-4-methylpiperazine
RN: **MP** (°C)**:**
MW: 266.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.962E-04	1.855E-01	25	M438	0 0 0 0 0	

3905. $C_{18}H_{22}N_4O_5$
Dis. A. 9
Ethanol, 2,2′-[[4-[(2-methoxy-4-nitrophenyl)azo]-3-methylphenyl]imino]*bis*-
4-[bis(2-Hydroxyethyl)amino]-2′-methoxy-2-methyl-4′-nitroazobenzene
RN: 41541-11-1 **MP** (°C)**:**
MW: 374.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-06	1.685E-03	25	B333	0 0 0 0 0	

3906. $C_{18}H_{22}O_2$
Hexestrol
4,4′-(1,2-Diethylethylene)diphenol
Dihydrodiethylstilbestrol
Esestrolo
RN: 5635-50-7 **MP** (°C)**:** 186.5
MW: 270.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.438E-05	1.200E-02	37	B039	2 1 1 1 0	EFG
3.699E-05	1.000E-02	37	B045	1 0 1 1 1	
4.365E-05	1.180E-02	ns	R427	0 0 0 0 0	

3907. $C_{18}H_{22}O_2$
Estrone
Oestrone
Folliculin
1,3,5(10)-Estratrien-3-ol-17-one
Estra-1,3,5(10)-Trien-17-one, 3-hydroxy-
Oestrin
RN: 53-16-7 **MP** (°C)**:** 252.5
MW: 270.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.659E-06	1.530E-03	22	Y419	0 0 0 0 0	
2.959E-06	8.000E-04	25	H049	0 0 0 0 0	
1.110E-04	3.000E-02	25	I309	0 0 0 0 0	*sic*
2.959E-06	8.000E-04	25	L033	1 0 2 1 1	
1.109E-03	2.999E-01	25	P324	0 0 0 0 0	
4.808E-06	1.300E-03	25	S468	0 0 0 0 0	
8.200E-06	2.217E-03	37	H034	1 0 2 1 1	pH 7.4
1.184E-05	3.200E-03	37	L010	2 0 2 1 1	
3.162E-06	8.550E-04	ns	A074	0 0 0 0 0	EFG

3908. $C_{18}H_{23}NO$
Orphenadrine
Disipal
Marflex
Noradex
Orflagen
Norflex
RN: 83-98-7 **MP** (°C)**:**
MW: 269.39 **BP** (°C)**:** 195 at 12 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-06	1.801E-03	22.5	B440	0 0 0 0 0	

3909. $C_{18}H_{23}N_3O_3S$
L-Leu-dapsone
2-Amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-4-methyl-, (*S*)-
Pentanamide
RN: 160349-00-8 **MP** (°C)**:**
MW: 361.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.576E-04	3.100E-01	25	P351	0 0 0 0 0	pH 7.4
>6.92E-02	>2.50E+01	25	P351	0 0 0 0 0	

3910. $C_{18}H_{23}N_3O_4S$
Phentolamine methanesulfonate
Vasomax
Regitine mesylate
Regitine methanesulfonate
RN: 65-28-1 **MP** (°C)**:** 177
MW: 377.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.979E+00	1.502E+03	30	D011	1 0 1 0 2	

3911. $C_{18}H_{24}I_3N_3O_9$
1,3-Benzenedicarboxamide, 5*RS*-[(2,3-dihydroxy-1-oxobutyl)amino]-*N*,*N*′-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-[*RS*-(*RS**,*S**)]-
RN: 77868-48-5 **MP** (°C)**:**
MW: 807.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-01	1.071E+02	25	P091	0 0 0 0 0	

3912. $C_{18}H_{24}N_4O_2$
2,5-Diaziridinyl-3,6-dipyrrolidino-1,4-benzoquinone
RN: 59886-43-0 **MP** (°C)**:** 160
MW: 328.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.522E-03	5.000E-01	rt	C317	0 0 0 0 0	

3913. $C_{18}H_{24}N_4O_2S$
2-Sulfanilamido-5,6,7,8,-tetrahydro-8-isopropyl-5-methyl-quinazoline
RN: 71119-36-3 **MP** (°C)**:** 185-187
MW: 360.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-05	2.400E-02	29	C049	0 0 0 0 0	

3914. $C_{18}H_{24}N_4O_2S$
2-Sulfanilamidobornylenepyrimidine
RN: **MP** (°C)**:** 276
MW: 360.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.322E-05	3.000E-02	29	C049	0 0 0 0 0	

3915. $C_{18}H_{24}N_4O_3S$
L-Lys-dapsone
Hexanamide, 2,6-diamino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)
RN: 160349-03-1 **MP** (°C)**:**
MW: 376.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	pH 7.4
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	

3916. $C_{18}H_{24}O_2$
Estradiol
17-β-Estradiol
Estradiol-17β
RN: 50-28-2 **MP** (°C)**:** 176
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.652E-05	4.500E-03	20	G072	1 2 2 1 2	

(*continued*)

3916. $C_{18}H_{24}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.689E-03	20	L077	1 2 2 2 1	
1.413E-05	3.850E-03	22	Y419	0 0 0 0 0	
2.566E-05	6.990E-03	23	B014	0 0 1 2 2	
7.413E-06	2.019E-03	25	B041	1 0 2 2 0	EFG
6.000E-07	1.634E-04	25	E014	2 2 2 1 1	pH 7.3
1.432E-05	3.900E-03	25	H049	0 0 0 0 0	
1.836E-05	5.000E-03	25	K003	2 1 1 1 1	
5.544E-06	1.510E-03	25	S468	0 0 0 0 0	
1.320E-05	3.596E-03	27.34	L077	1 2 2 2 2	
2.060E-05	5.611E-03	35	L077	1 2 2 2 2	
1.500E-05	4.086E-03	37	H034	1 0 2 1 2	pH 7.4
2.350E-05	6.401E-03	37	H035	1 1 1 1 2	pH 7.4
1.430E-05	3.895E-03	37	H054	0 0 0 0 0	
1.880E-05	5.120E-03	37	R069	0 0 0 0 0	pH 7.4
1.000E-05	2.724E-03	37.50	B041	1 0 2 2 0	EFG
2.830E-05	7.709E-03	42	L077	1 2 2 2 2	
3.560E-05	9.697E-03	50	L077	1 2 2 2 2	

3917. $C_{18}H_{24}O_2$

α-Estradiol
17-α-Estradiol

RN: 57-91-0 **MP** (°C)**:** 220
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.432E-05	3.900E-03	25	L033	1 0 2 1 2	

3918. $C_{18}H_{24}O_3$

Estriol
Oestriol
Drihydroxyestrin

RN: 50-27-1 **MP** (°C)**:** 284.5
MW: 288.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	3.020E-02	22	Y419	0 0 0 0 0	
1.110E-05	3.200E-03	25	H049	0 0 0 0 0	
1.000E-04	2.884E-02	30	O321	0 0 0 0 0	
1.006E-04	2.900E-02	30	O321	0 0 0 0 0	

3919. $C_{18}H_{24}O_6$
Butylphthalyl butyl glycolate
1,2-Benzenedicarboxylic acid 2-butoxy-2-oxoethyl butyl ester
Butyl carbobutoxymethyl phthalate
RN: 85-70-1 **MP** (°C)**:** <–35
MW: 336.39 **BP** (°C)**:** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.567E-05	1.200E-02	20	F070	1 0 0 0 2	

3920. $C_{18}H_{25}I_3N_3O_9$
3,5-Diacetylamino-2,4,6-triiodobenzoic acid methyl-glucamide
RN: **MP** (°C)**:** 191
MW: 808.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.101E+00	8.900E+02	20	L100	1 0 0 0 1	

3921. $C_{18}H_{25}NO$
Racemethorphan
Dextromethorphan HBr
RN: 510-53-2 **MP** (°C)**:**
MW: 271.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-01	3.600E+01	37	F008	1 1 2 2 2	0.1N HCl

3922. $C_{18}H_{25}NO$
Dextromethorphan
(+)-*cis*-1,3,4,9,10,10a-Hexahydro-6-methoxy-11-methyl-2H-10,4a-iminoethanophenanthrene
Romilar CF
DXM Free Base
3-Methoxy-17-methyl-(9α,13α,14α)-morphinan
Benylin DM
RN: 125-71-3 **MP** (°C)**:**
MW: 271.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.316E-04	9.000E-02	amb	L434	0 0 0 0 0	

3923. $C_{18}H_{25}NO_5S_2$

Methyl *N*-{5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: **MP** (°C)**:**

MW: 399.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.003E-05	1.200E-02	ns	S453	0 0 0 0 0	

3924. $C_{18}H_{25}N_3O_2$

2-Ethoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide

N-[2-(Diethylamino)ethyl]-2-ethoxyquinoline-4-carboxamide

RN: 2716-99-6 **MP** (°C)**:**

MW: 315.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-04	2.082E-01	ns	M066	0 0 0 0 1	

3925. $C_{18}H_{26}NO_4$

Ibuprofen *N*-methyl-*N*-carbamoyl methyl glycolamide ester

RN: **MP** (°C)**:** 100.5

MW: 320.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.057E-04	1.300E-01	0	B331	1 2 2 1 1	pH 7.4

3926. $C_{18}H_{26}N_2O_4$

Benzeneacetic acid, β-methyl-4-(2-methylpropyl)-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxo-ethyl ester

Ibuprofen *N*-methyl-*N*-carbamoyl methyl glycolamide ester

RN: 114665-11-1 **MP** (°C)**:** 100–101

MW: 334.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	1.300E-01	21	B331	0 0 0 0 0	

3927. $C_{18}H_{26}N_4O_6$

9-[5-*O*-(Heptylate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 142963-79-9 **MP** (°C)**:** foam

MW: 394.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-04	8.362E-02	37	M378	1 2 1 1 2	pH 7.2

3928. $C_{18}H_{26}N_4O_6.0.5H_2O$

2′-Heptanyl-6-methoxypurine arabinoside (hemihydrate)
RN: 145913-40-2 **MP** (°C)**:** 83–85
MW: 403.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-03	1.122E+00	37	C348	0 0 0 0 0	pH 7.00

3929. $C_{18}H_{26}O$

Acetyl ethyl tetramethyl tetralin
1-(3-Ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)ethanone
AETT
1,1,4,4-Tetramethyl-6-ethyl-7-acetyl-1,2,3,4-tetrahydronaphthalene
Ethanone, 1-(3-ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl)-
RN: 88-29-9 **MP** (°C)**:**
MW: 258.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-08	1.200E-05	ns	B338	0 0 0 0 1	

3930. $C_{18}H_{26}O_2$

Nortestosterone
Estr-4-en-3-one, 17-hydroxy-, (17β)
RN: 434-22-0 **MP** (°C)**:**
MW: 274.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-02	3.090E+00	25	P324	0 0 0 0 0	

3931. $C_{18}H_{26}O_4$

Dipentyl phthalate
Diamyl phthalate
RN: 131-18-0 **MP** (°C)**:** <–55
MW: 306.41 **BP** (°C)**:** 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E-06	4.443E-04	20	L300	2 1 0 2 2	
9.791E-07	3.000E-04	25	F067	1 0 2 2 0	
3.263E-04	9.999E-02	ns	F014	0 0 0 0 0	

3932. $C_{18}H_{26}O_6$
Butyl phthalyl butyl glycollate
RN: **MP** (°C)**:**
MW: 338.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.955E-05	1.000E-02	15	H069	1 0 1 1 0	
5.318E-04	1.800E-01	ns	F014	0 0 0 0 1	

3933. $C_{18}H_{27}NO$
N-Nonylcinnamamide
2-Propenamide, *N*-nonyl-3-phenyl-
RN: 59832-01-8 **MP** (°C)**:**
MW: 273.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-06	6.070E-04	ns	H350	0 0 0 0 0	

3934. $C_{18}H_{27}NO_3$
p-Acetamidophenyl decanoate
Acetaminophen decanoate
RN: 54942-37-9 **MP** (°C)**:** 107
MW: 305.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.947E-05	9.000E-03	25	B010	1 1 1 1 0	

3935. $C_{18}H_{27}NO_3$
Capsaicin
Nonenamide, *N*-((4-hydroxy-3-methoxyphenyl)methyl)-8-methyl-, (E)-
Zostrix
RN: 404-86-4 **MP** (°C)**:** 63 C
MW: 305.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.176E-02	27	Z412	0 0 0 0 0	

3936. $C_{18}H_{27}N_5O_5$
9-[5′-(*O*-Caprylyl)-β-D-arabinofuranosyl]adenine ester
RN: 66460-51-3 **MP** (°C)**:**
MW: 393.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-04	1.000E-01	ns	B134	0 1 1 1 0	

3937. $C_{18}H_{28}N_2O$

DL-Bupivacaine
Bupivacaine
Marcaine
Bupivicaine
Marcaine (hydrochloride monohydrate)

RN: 2180-92-9 **MP** (°C)**:** 107
MW: 288.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	1.082E-01	14.9	N046	2 0 1 1 2	intrinsic
9.025E-06	2.603E-03	22.5	B440	0 0 0 0 0	
1.733E-03	5.000E-01	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
3.520E-04	1.015E-01	25	D401	1 2 2 2 2	
3.180E-04	9.172E-02	25	N046	2 0 1 1 2	intrinsic
3.130E-04	9.028E-02	34.5	N046	2 0 1 1 2	intrinsic
4.170E-04	1.203E-01	37	N044	2 1 1 2 2	intrinsic

3938. $C_{18}H_{28}N_4O_2$

2,5-Diaziridinyl-3,6-bis(butylamino)-1,4-benzoquinone

RN: 59886-48-5 **MP** (°C)**:** 95
MW: 332.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.01E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3939. $C_{18}H_{28}O_3$

Undecyl *p*-hydroxybenzoate
Undecyl 4-hydroxybenzoate

RN: 69679-31-8 **MP** (°C)**:**
MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.079E-03	2.362E+00	25	D081	1 2 2 1 2	

3940. $C_{18}H_{29}NO_2$

Penbutolol
Levatol
2-Propanol, 1-(2-cyclopentylphenoxy)-3-[(1,1-dimethylethyl)amino]-, (*S*)-

RN: 38363-40-5 **MP** (°C)**:** 70
MW: 291.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.402E-02	7.000E+00	rt	H096	1 0 0 0 0	

3941. $C_{18}H_{29}NO_3$
4-Pentoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-73-8 **MP** (°C)**:**
MW: 307.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.845E-02	ns	M066	0 0 0 0 1	

3942. $C_{18}H_{30}$
2-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3943. $C_{18}H_{30}$
4-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3944. $C_{18}H_{30}$
5-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3945. $C_{18}H_{30}$
3-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	1.725E-06	25	S377	0 0 0 0 0	

3946. $C_{18}H_{30}$
6-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3947. $C_{18}H_{30}N_2O_2$
4-Pentylaminobenzoic acid-2-(diethylamino)ethyl ester
RN: 16488-56-5 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.435E-02	ns	M066	0 0 0 0 1	

3948. $C_{18}H_{30}O_3$
4-Octylphenol diethoxylate
2-[2-(*p*-Octylphenoxy)ethoxy]ethanol
RN: 51437-90-2 **MP** (°C)**:**
MW: 294.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.483E-05	1.320E-02	20.5	A335	0 0 0 0 0	
4.490E-05	1.322E-02	20.5	A335	0 0 0 0 0	

3949. $C_{18}H_{30}O_{15}.4H_2O$
Triamylose (tetrahydrate)
RN: **MP** (°C)**:**
MW: 558.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.298E-02	1.283E+01	20	P048	1 2 1 1 1	

3950. $C_{18}H_{31}NO_4$
Bisoprolol
1-[Isopropylamino]-3-[isopropoxyethoxymethylphenoxy]-2-propanol
ZEβ
Ziac
RN: 66722-44-9 **MP** (°C)**:**
MW: 325.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-08	5.500E-06	100	M418	0 0 0 0 0	

3951. $C_{18}H_{31}O_4P$

Butyl octyl phenyl phosphate

RN: 110459-55-7 **MP** (°C)**:**
MW: 342.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

3952. $C_{18}H_{32}O_7$

Tributyl citrate
Tri-*n*-butyl citrate
Butyl citrate

RN: 77-94-1 **MP** (°C)**:** –20
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.664E-04	6.000E-02	15	H069	1 0 1 1 0	
2.219E-04	7.999E-02	ns	F014	0 0 0 0 0	

3953. $C_{18}H_{32}O_{16}$

Raffinose
6G-α-D-Galactosylsucrose
Melitose
Gossypose
Melitriose

RN: 512-69-6 **MP** (°C)**:** 80.0
MW: 504.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.556E-02	3.307E+01	.02	H040	1 2 2 2 2	
1.227E-01	6.191E+01	10.00	H040	1 2 2 2 1	
1.879E-01	9.478E+01	16.38	H040	1 2 2 2 2	
1.937E-01	9.772E+01	16.90	H040	1 2 2 2 2	
2.480E-01	1.251E+02	20	D041	1 0 0 0 2	
2.373E-01	1.197E+02	20.00	H040	1 2 2 2 2	
3.192E-01	1.610E+02	24.80	H040	1 2 2 2 2	
4.555E-01	2.298E+02	25	P049	1 0 1 1 1	
3.228E-01	1.628E+02	25.05	H040	1 2 2 2 2	
3.340E-01	1.685E+02	25.50	H040	1 2 2 2 2	
4.227E-01	2.132E+02	30.00	H040	1 2 2 2 2	
6.398E-01	3.227E+02	39.38	H040	1 2 2 2 2	
6.599E-01	3.329E+02	40.00	H040	1 2 2 2 2	
9.217E-01	4.650E+02	50.00	H040	1 2 2 2 2	
1.016E+00	5.125E+02	53.20	H040	1 2 2 2 2	
1.201E+00	6.060E+02	60.00	H040	1 2 2 2 2	
1.239E+00	6.250E+02	61.60	H040	1 2 2 2 2	
1.473E+00	7.430E+02	70.00	H040	1 2 2 2 2	

(*continued*)

3953. $C_{18}H_{32}O_{16}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E+00	8.484E+02	78.00	H040	1 2 2 2 2	
6.518E-02	3.288E+01	.00	H040	1 2 2 2 1	
2.480E-01	1.251E+02	rt	D021	0 0 1 1 2	

3954. $C_{18}H_{32}O_{16}.5H_2O$

Raffinose (pentahydrate)
6G-α-D-Galactosylsucrose (pentahydrate)
RN: 17629-30-0 **MP** (°C)**:** 80
MW: 594.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.531E-02	3.288E+01	0	M043	1 0 0 0 1	
1.041E-01	6.191E+01	10	M043	1 0 0 0 1	
2.014E-01	1.197E+02	20	M043	1 0 0 0 2	
3.586E-01	2.132E+02	30	M043	1 0 0 0 2	
5.599E-01	3.329E+02	40	M043	1 0 0 0 2	
7.821E-01	4.650E+02	60	M043	1 0 0 0 2	
1.019E+00	6.060E+02	80	M043	1 0 0 0 2	

3955. $C_{18}H_{34}OSn$

Cyhexatin
Tricyclohexylhydroxystannane
Tricyclohexyltin hydroxide
Plictran
Dowco 213
RN: 13121-70-5 **MP** (°C)**:** 196.5
MW: 385.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.60E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.60E-06	<1.00E-03	ns	K138	0 0 0 0 1	

3956. $C_{18}H_{34}O_4$

Dibutyl sebacate
Di-*n*-butyl sebacate
Decanedioic acid dibutyl ester
Dibutyl decanedioate
RN: 109-43-3 **MP** (°C)**:**
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-04	5.000E-02	ns	F014	0 0 0 0 0	

3957. $C_{18}H_{36}O_2$

Stearic acid
Stearinsaeure
Octadecanoic acid

RN: 57-11-4 **MP** (°C)**:** 70
MW: 284.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.327E-06	1.800E-03	0	B136	1 0 2 1 1	
9.842E-06	2.800E-03	20	B136	1 0 2 1 1	
1.055E-05	3.000E-03	20	F300	1 0 0 0 0	
1.019E-05	2.900E-03	20.0	R001	1 1 1 1 1	
2.100E-06	5.974E-04	25	J001	1 0 2 1 1	
1.970E-06	5.604E-04	25	R002	0 0 0 0 0	
1.195E-05	3.400E-03	30	B136	1 0 2 1 1	
1.195E-05	3.400E-03	30.0	R001	1 1 1 1 1	
1.700E-05	4.836E-03	35	M004	2 0 0 0 2	
1.476E-05	4.200E-03	45	B136	1 0 2 1 1	
1.476E-05	4.200E-03	45.0	R001	1 1 1 1 1	
2.700E-06	7.681E-04	50	J001	1 0 2 1 1	
5.770E-05	1.641E-02	50	M004	2 0 0 0 2	
1.758E-05	5.000E-03	60	B136	1 0 2 1 1	
1.758E-05	5.000E-03	60	F300	1 0 0 0 0	
1.758E-05	5.000E-03	60.0	R001	1 1 1 1 1	
1.145E-05	3.257E-03	62.5	M004	1 0 0 0 2	
6.327E-06	1.800E-03	.0	R001	1 1 1 1 1	

3958. $C_{18}H_{38}$

n-Octadecane
Octadecane

RN: 593-45-3 **MP** (°C)**:** 29.5
MW: 254.50 **BP** (°C)**:** 317.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-07	1.200E-04	10	C331	0 0 0 0 0	
2.358E-08	6.000E-06	25	B069	1 0 1 1 1	
2.240E-08	5.700E-06	25	B069	1 0 1 1 1	
5.894E-07	1.500E-04	30	C331	0 0 0 0 0	
6.680E-07	1.700E-04	60	C331	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B003	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B033	0 0 0 0 2	

3959. $C_{18}H_{38}O$

Octadecanol
Stearyl alcohol
Octadecyl alcohol
Steraffine

RN: 112-92-5 **MP** (°C)**:** 61
MW: 270.50 **BP** (°C)**:** 336

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.082E-06	34	K011	1 2 1 1 1	
2.200E-08	5.951E-06	65	K011	1 2 1 1 1	

3960. $C_{18}H_{39}N.2H_2O$

Octadecylamine (dihydrate)
1-Aminooctadecane (dihydrate)

RN: 124-30-1 **MP** (°C)**:**
MW: 305.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.891E-09	1.800E-06	ns	R037	0 2 2 1 1	

3961. $C_{18}H_{39}O_3P$

Dibutyl decyl phosphonate

RN: 36378-71-9 **MP** (°C)**:**
MW: 334.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.00E-01	25	B070	1 2 0 1 0	

3962. $C_{18}H_{39}O_4P$

Dibutyl decyl phosphate

RN: 111440-78-9 **MP** (°C)**:**
MW: 350.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-04	<1.00E-01	25	B070	1 2 0 1 0	

3963. $C_{18}H_{39}O_7P$

Tributoxyethyl phosphate

RN: 78-51-3 **MP** (°C)**:** –70
MW: 398.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-03	1.100E+00	25	B070	1 2 0 1 1	

3964. $C_{19}H_{12}O_6$
Dicumarol
3,3′-Methylene-bis(4-hydroxycoumarin)
Dicoumarol
RN: 66-76-2 **MP** (°C)**:** 290
MW: 336.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.352E-05	1.800E-02	25	M457	0 0 0 0 0	
<4.46E-04	<1.50E-01	25	P312	0 0 0 0 0	

3965. $C_{19}H_{13}Cl$
6-Chloro-10-methyl-1,2-benzanthracene
RN: 188124-97-2 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.613E-08	1.000E-05	27	D003	1 0 0 1 0	

3966. $C_{19}H_{13}Cl$
4-Fluoro-10-methyl-1,2-benzanthracene
4-FMBA
RN: 2990-70-7 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3967. $C_{19}H_{13}Cl$
3-Fluoro-10-methyl-1,2-benzanthracene
3-FMBA
RN: 20629-50-9 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3968. $C_{19}H_{14}$
10-Methyl-1,2-benzanthracene
RN: 2541-69-7 **MP** (°C)**:** 141
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.539E-08	1.100E-05	24	H116	2 1 0 0 1	

3969. $C_{19}H_{14}$
1′-Methyl-1,2-benzanthracene
RN: 2498-77-3 **MP** (°C)**:** 138
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E-07	5.500E-05	27	D003	1 0 0 1 2	

3970. $C_{19}H_{14}$
5-Methylchrysene
RN: 3697-24-3 **MP** (°C)**:** 117.1
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-07	6.200E-05	27	D003	1 0 0 1 1	

3971. $C_{19}H_{14}$
9-Methyl-1,2-benzanthracene
RN: 2381-16-0 **MP** (°C)**:** 138
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.527E-07	3.700E-05	24	H116	2 1 0 0 1	

3972. $C_{19}H_{14}$
6-Methylchrysene
RN: 1705-85-7 **MP** (°C)**:** 149
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-07	6.500E-05	27	D003	1 0 0 1 1	

3973. $C_{19}H_{14}O_3$
Aurin
Rosolic acid
4-[*bis*-(*p*-Hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one
RN: 603-45-2 **MP** (°C)**:**
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-03	1.199E+00	rt	D021	0 0 1 1 1	

3974. $C_{19}H_{14}O_5S$
Phenolsulfonaphthalein
Phenolrot
RN: 143-74-8 **MP** (°C)**:** >300
MW: 354.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.748E-04	3.100E-01	100	F300	1 0 0 0 2	

3975. $C_{19}H_{16}O$
Triphenylcarbinol
Triphenylmethanol
RN: 76-84-6 **MP** (°C)**:** 164.2
MW: 260.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.432E+00	25	D007	2 0 1 1 2	

3976. $C_{19}H_{17}ClN_2O$
Prazepam
Centrax
7-Chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one
Demetrin
Verstran
RN: 2955-38-6 **MP** (°C)**:**
MW: 324.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	9.095E-03	25	M320	2 2 1 1 2	
		amb	L434	0 0 0 0 0	

3977. $C_{19}H_{17}ClN_2O_4$
Quizalofop-ethyl
Quizalofop-et
Quizalofop ethyl ester
Targa
Pilot
NC 302
RN: 76578-14-8 **MP** (°C)**:** 91.7–92.1
MW: 372.81 **BP** (°C)**:** 220 at 0.2 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.128E-07	3.030E-04	ns	R427	0 0 0 0 0	

3978. $C_{19}H_{17}ClN_2O_4$
Glafenine
N-(7-Chloro-4-quinolyl)anthranilate
2,3-Dihydroxypropyl-*N*-(7-chloro-4-quinolinyl)anthranilate
RN: 3820-67-5 **MP** (°C)**:** 169.5
MW: 372.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-01	3.846E+01	ns	M152	0 0 0 0 0	pH 1.0, intrinsic

3979. $C_{19}H_{17}ClN_4$
Fenbuconazole
α-(2-(4-Chlorophenyl)ethyl)-α-phenyl-1H-1,2,4-triazole-1-propanenitrile
Enable
RH-7592
Fenethanil
1,2,4-Triazole-1-propanenitrile, α-{2-(4-chlorophenyl)ethyl}-α-phenyl
RN: 114369-43-6 **MP** (°C)**:**
MW: 336.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-07	1.983E-04	ns	R427	0 0 0 0 0	

3980. $C_{19}H_{17}N_3O_4S_2$
Sugordomycin
RN: 1405-50-1 **MP** (°C)**:**
MW: 415.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.304E-02	9.572E+00	21	M044	2 0 2 2 2	

3981. $C_{19}H_{17}N_3O_4S_2$
Cephaloridine
Glaxoridin
Keflodin
Loridine
RN: 50-59-9 **MP** (°C)**:** 184
MW: 415.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.81E-02	>2.00E+01	21	M044	2 0 2 2 0	

3982. $C_{19}H_{17}N_3O_5$
1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, ethyl ester
RN: 153474-30-7 **MP** (°C)**:** 165.5
MW: 367.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.722E-05	1.000E-02	21	N337	0 0 0 0 0	pH 5
2.700E-05	9.919E-03	21	N337	0 0 0 0 0	pH 5

3983. $C_{19}H_{18}$
1,2,3,4-Tetrahydro-10-methyl-1,2-benzanthracene
10-Methyl-1,2-cyclohexane anthracene
RN: 6366-18-3 **MP** (°C)**:** 117
MW: 246.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.786E-07	4.400E-05	27	D003	1 0 0 1 1	

3984. $C_{19}H_{18}Cl_2N_2O_2$
G-20
p,*p*-Dichlorophenylbutazone
RN: 4047-57-8 **MP** (°C)**:**
MW: 377.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.386E-04	9.000E-02	ns	B158	0 0 0 0 1	pH 7.0

3985. $C_{19}H_{18}N_2O_3$
G-23
1-Oxybutylphenylbutazone
3,5-Pyrazolidinedione, 4-butyryl-1,2-diphenyl-
RN: 13167-98-1 **MP** (°C)**:**
MW: 322.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.722E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3986. $C_{19}H_{18}N_2O_3$
Kebuzone
3,5-Pyrazolidinedione
RN: 853-34-9 **MP** (°C)**:** 128
MW: 322.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.402E-04	1.742E-01	20	M140	2 0 1 1 1	

3987. $C_{19}H_{19}ClFNO_3$

Flamprop-isopropyl
Flufenprop-isopropyl
Isopropyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)alanine
1-Methylethyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-DL-alanine
RN: 52756-22-6 **MP** (°C)**:** 56.5
MW: 363.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-05	1.800E-02	20	M161	1 0 0 0 0	

3988. $C_{19}H_{19}N_7O_6$

Folic acid
N-(*p*-(((2-Amino-4-hydroxy-6-pteridinyl)methyl)amino)benzoyl)-L-glutamic acid
Vitamin M
Pteroylglutamic acid
Folcysteine
Folacin
RN: 59-30-3 **MP** (°C)**:**
MW: 441.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-03	1.597E+00	25	D041	1 0 0 0 1	*sic*
3.625E-06	1.600E-03	25	D315	0 0 0 0 0	
2.243E-02	9.901E+00	100	D041	1 0 0 0 0	*sic*
2.265E-04	1.000E-01	ns	K444	0 0 0 0 0	

3989. $C_{19}H_{20}ClNO_9$

Griseofulvin-4-carboxy-methoxime
RN: **MP** (°C)**:**
MW: 441.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.704E-04	7.529E-02	37	F033	2 0 2 0 2	

3990. $C_{19}H_{20}F_3NO_4$

Fluazifop-butyl
Butyl 2-(4-((5-trifluoromethyl-2-pyridinyl)oxy)phenoxy)propanoate
Onecide
Fluazifop-butyl
Fluazifop butyl ester
Hache uno super
RN: 69806-50-4 **MP** (°C)**:** 13
MW: 383.37 **BP** (°C)**:** 165 at 2.02 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	5.366E-04	ns	S460	0 0 0 0 0	

3991. $C_{19}H_{20}N_2O$

Cinchoninone
Cinchoninon
9-Deoxy-9-oxocinchonine
RN: 14509-68-3 **MP** (°C)**:**
MW: 292.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.498E-04	1.900E-01	20	F300	1 0 0 0 1	

3992. $C_{19}H_{20}N_2O_2$

Phenylbutazone
1,2-Diphenyl-4-butyl-3,5-dioxopyrazolidine
Butazolidin
Equiphen
Butazone
RN: 50-33-9 **MP** (°C)**:** 107
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-05	2.595E-02	20	H301	0 0 0 0 0	
4.864E-05	1.500E-02	20	P026	1 0 1 1 1	
1.102E-04	3.400E-02	25	P096	0 0 0 0 0	
1.540E-04	4.750E-02	30	D015	2 0 1 1 0	EFG
1.000E-03	3.084E-01	35	H091	1 2 2 2 1	*sic*
9.076E-03	2.799E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
7.575E-03	2.336E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
9.362E-03	2.887E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
6.907E-03	2.130E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
2.108E-04	6.500E-02	37	D015	2 0 1 1 0	EFG
1.816E-04	5.600E-02	37	E047	1 0 1 1 1	
7.134E-03	2.200E+00	ns	B158	0 0 0 0 1	pH 7.0
1.037E-03	3.199E-01	ns	B404	0 2 1 1 0	
1.300E-04	4.009E-02	ns	O304	0 0 1 2 2	
2.594E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic
1.310E-01	4.040E+01	rt	N056	0 0 1 1 2	average of 2

3993. $C_{19}H_{20}N_2O_2$

G-21
p,*p*-Dimethylphenylbutazone
RN: 745-27-7 **MP** (°C)**:**
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.891E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3994. $C_{19}H_{20}N_2O_3$

Oxyphenbutazone
p-Hydroxyphenylbutazone
RN: 129-20-4 **MP** (°C)**:** 124
MW: 324.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	6.000E-02	30	D015	2 0 1 1 0	EFG
2.497E-04	8.100E-02	37	D015	2 0 1 1 0	EFG
3.083E-02	1.000E+01	ns	B158	0 0 0 0 1	pH 7.0, *sic*
>1.54E-03	>5.00E-01	ns	B404	0 2 1 1 0	
6.166E-05	2.000E-02	rt	H302	0 0 2 1 2	intrinsic

3995. $C_{19}H_{20}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-[4-methylbenzoyl]-β-D-arabinofuranosyl)-9H-purine (hemihydrate)
RN: 121032-20-0 **MP** (°C)**:** 127–128
MW: 409.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-05	1.433E-02	37	M378	1 2 1 1 2	pH 7.2

3996. $C_{19}H_{20}N_4O_6$

2′-(*p*-Toluylyl)-6-methoxypurine arabinoside
2′-Phenylacetyl-6-methoxypurine arabinoside
RN: 121032-52-8 **MP** (°C)**:** 69–73
MW: 400.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.870E-02	2.350E+01	37	C348	0 0 0 0 0	pH 7.00
5.840E-03	2.338E+00	37	C348	0 0 0 0 0	pH 7.00

3997. $C_{19}H_{20}N_4O_6.0.1H_2O$

9-[5-*O*-(Benzyl formyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.1 hydrate)

RN: 121032-36-8 **MP** (°C)**:** foam
MW: 402.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-02	4.223E+00	37	M378	1 2 1 1 2	pH 7.2

3998. $C_{19}H_{20}N_4O_7$

2′-(*p*-Methoxybenzoyl)-6-methoxypurine arabinoside

RN: 121032-51-7 **MP** (°C)**:** 71–75
MW: 416.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-03	2.773E+00	37	C348	0 0 0 0 0	pH 7.00

3999. $C_{19}H_{20}N_4O_7.0.5H_2O$

2′-Phenoxyacetyl-6-methoxypurine arabinoside (hemihydrate)

RN: 145913-46-8 **MP** (°C)**:** 123–125
MW: 425.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.21E-02	>9.40E+00	37	C348	0 0 0 0 0	pH 7.00

4000. $C_{19}H_{20}N_4O_7.0.25H_2O$

9-[5-*O*-(4-Methoxybenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)

RN: 121032-35-7 **MP** (°C)**:** 195–197
MW: 420.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	8.250E-02	37	M378	1 2 1 1 2	pH 7.2

4001. $C_{19}H_{20}N_4O_7.0.05H_2O$

9-[5-*O*-(Benzyl acetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.05 hydrate)

RN: 121032-37-9 **MP** (°C)**:** 193-195
MW: 417.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.930E-04	1.640E-01	37	M378	1 2 1 1 2	pH 7.2

4002. $C_{19}H_{20}O_4$
Butylbenzyl phthalate
Butyl phenyl-methyl phthalate
Benzylbutyl phthalate
Phthalate butyl benzyl ester
Butyl benzyl phthalate
1,2-Benzenedicarboxylic acid butyl phenylmethyl ester
RN: 85-68-7 **MP** (°C)**:** <–35
MW: 312.37 **BP** (°C)**:** 370

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.020E-06	2.818E-03	20	L300	2 1 0 2 2	
3.778E-05	1.180E-02	22	Y419	0 0 0 0 0	
2.273E-06	7.100E-04	24	H116	2 1 0 0 2	
8.644E-06	2.700E-03	25	F067	1 0 2 2 1	

4003. $C_{19}H_{21}ClO_4$
Isobutyl (+/–)-2-[4-(4-chlorophenoxy)phenoxy]propionate
RN: 51337-71-4 **MP** (°C)**:** 39.5
MW: 348.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.160E-04	1.800E-01	22	M161	1 0 0 0 2	

4004. $C_{19}H_{21}F_3N_2S$
2-Trifluoromethyl-*N*,*N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 2340-66-1 **MP** (°C)**:**
MW: 366.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.832E-03	ns	G023	0 0 1 1 0	

4005. $C_{19}H_{21}NO$
Doxepin
Adapin
Deptran
Sinequan
RN: 1668-19-5 **MP** (°C)**:** 120
MW: 279.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-04	3.157E-02	25	E051	1 0 2 1 2	

4006. $C_{19}H_{21}NO_3$
Thebaine
Paramorphine
Morphinan, 6,7,8,14-tetradehydro-4,5α-epoxy-3,6-dimethoxy-17-methyl-
RN: 115-37-7 **MP** (°C)**:**
MW: 311.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	6.850E-01	15	K059	2 2 2 0 1	

4007. $C_{19}H_{21}N_3O$
Zolpidem
RN: 82626-48-0 **MP** (°C)**:**
MW: 307.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.25E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4008. $C_{19}H_{21}N_5O_2$
Dis. A. 6
Propanenitrile, 3-[butyl[4-[(4-nitrophenyl)azo]phenyl]amino]-
RN: 69472-19-1 **MP** (°C)**:** 118
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-08	7.028E-06	25	B333	0 0 0 0 0	

4009. $C_{19}H_{21}N_5O_2$
Dye VII
4-[[(4-(*N*-Butyl-*N*-ethylnitrile)amino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-07	1.687E-04	71.80	B198	1 2 1 1 1	
9.700E-07	3.409E-04	84.10	B198	1 2 1 1 1	
2.020E-06	7.099E-04	97.40	B198	1 2 1 1 2	

4010. $C_{19}H_{21}N_5O_4$
Prazosin
Minipress
Pressin
RN: 19216-56-9 **MP** (°C)**:**
MW: 383.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.346E-06	3.200E-03	22.5	B422	0 0 0 0 0	

4011. $C_{19}H_{21}N_5O_5$
9-[5′-(*O*-Hydrocinnamoyl)-β-D-arabinofuranosyl]adenine ester
RN: 68325-41-7 **MP** (°C)**:**
MW: 399.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.756E-03	1.500E+00	ns	B134	0 1 1 1 1	

4012. $C_{19}H_{22}Cl_2O_2$
1-Methyl-1,1-dichloro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-23-7 **MP** (°C)**:**
MW: 353.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-07	5.000E-05	rt	C122	0 0 0 0 0	

4013. $C_{19}H_{22}N_2O$
Cinchonidine
Cinchonidin
(8α,9*R*)-Cinchonan-9-ol
L-Cinchonidine
RN: 485-71-2 **MP** (°C)**:** 210
MW: 294.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.650E-01	15	K059	2 2 2 0 0	
9.511E-05	2.800E-02	22	M459	0 0 0 0 0	
6.793E-04	2.000E-01	25	F300	1 0 0 0 0	
1.970E-03	5.800E-01	100	F300	1 0 0 0 1	
6.792E-04	2.000E-01	c	D004	0 0 0 0 0	
8.490E-04	2.499E-01	rt	D021	0 0 1 1 1	

4014. $C_{19}H_{22}N_2O$
Cinchonine
Cinchonan-9-ol
(+)-Cinchonine
(9S)-Cinchonan-9-ol
RN: 118-10-5 **MP** (°C)**:** 265
MW: 294.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-06	1.413E-03	15	K059	2 2 2 0 1	
2.378E-05	7.000E-03	22	M459	0 0 0 0 0	
9.253E-04	2.724E-01	25	D004	0 0 0 0 0	
9.171E-04	2.700E-01	100	F300	1 0 0 0 1	
8.150E-04	2.399E-01	rt	D021	0 0 1 1 1	

4015. $C_{19}H_{22}N_2OS$
Acetylpromazine
3-Acetyl-10-(3-dimethylaminopropyl)phenothiazine
Plegicil
Vetranquil
Notensil
Plivafen
RN: 61-00-7 **MP** (°C)**:**
MW: 326.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.901E-05	1.600E-02	25	L045	1 1 1 1 2	intrinsic

4016. $C_{19}H_{22}N_2O_5$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester
Naproxen *N*-methyl-*N*-carbamoyl methyl glycolamide ester
RN: 114681-69-5 **MP** (°C)**:** 179
MW: 358.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-04	5.900E-02	21	B331	0 0 0 0 0	

4017. $C_{19}H_{22}N_2S$
Mepazine
Pecazine
RN: 60-89-9 **MP** (°C)**:** 80
MW: 310.46 **BP** (°C)**:** 233

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-05	5.588E-03	24	G022	2 0 1 1 1	

4018. $C_{19}H_{23}ClO_2$
1-Chloro-1-methyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-22-6 **MP** (°C)**:**
MW: 318.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-06	8.800E-04	rt	C122	0 0 0 0 0	

4019. $C_{19}H_{23}NO_3$
Ethylmorphine
7,8-Didehydro-4,5-epoxy-3-ethoxy-17-methylmorphinan-6-ol
RN: 76-58-4 **MP** (°C)**:**
MW: 313.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.916E-03	2.794E+00	20	K052	1 1 1 1 2	

4020. $C_{19}H_{23}NO_4$
1-Methyl-1-nitro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 26258-70-8 **MP** (°C)**:**
MW: 329.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.093E-06	3.600E-04	rt	C122	0 0 0 0 0	

4021. $C_{19}H_{23}NO_5$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl ester
Naproxen *N*-methyl-*N*-ethanol glycolamide ester
RN: 114665-19-9 **MP** (°C)**:** 110
MW: 345.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.053E-04	1.400E-01	21	B331	0 0 0 0 0	

4022. $C_{19}H_{23}N_3$
Amitraz
1,5-Di(2,4-dimethylphenyl)-3-methyl-1,3,5-triazapenta-1,4-diene
Ovasyn
Mitac
Triazid
Baam
RN: 33089-61-1 **MP** (°C)**:** 86.5
MW: 293.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-06	1.000E-03	rt	M161	0 0 0 0 0	

4023. $C_{19}H_{23}N_3O_2$
Ergonovine
9,10-Didehydro-*N*-(2-hydroxy-1-methylethyl)-6-methylergoline-8-carboxamide
Ergometrine
RN: 60-79-7 **MP** (°C)**:**
MW: 325.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.21E+00	>3.94E+02	25	B443	0 0 0 0 0	

4024. $C_{19}H_{23}N_5O_4$
Benzoic acid, 4-[(dimethylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-68-6 **MP** (°C)**:**
MW: 385.43 **BP** (°C)**:** 651.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.373E-03	1.300E+00	21	B419	1 1 2 2 1	int

4025. $C_{19}H_{24}N_2$
1-(Diphenylmethyl)-4-ethylpiperazine
RN: **MP** (°C)**:**
MW: 280.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	5.693E-01	25	M438	0 0 0 0 0	

4026. $C_{19}H_{24}N_2$
Imipramine
10,11-Dihydro-*N*,*N*-dimethyl-5H-dibenz[b,f]azepine-5-propanamine
5-[3-(Dimethylamino)propyl]-10,11-dihydro-5H-dibenz[b,f]azepine
RN: 50-49-7 **MP** (°C)**:** 174
MW: 280.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.823E-02	24	G022	2 0 1 1 1	

4027. $C_{19}H_{24}N_2O$
Hydrocinchonine
Hydrocinchonin
Cinchotine
RN: 485-65-4 **MP** (°C)**:** 268
MW: 296.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.362E-03	7.000E-01	16	F300	1 0 0 0 1	
2.593E-03	7.686E-01	25	D004	0 0 0 0 0	

4028. $C_{19}H_{24}N_2OS$
Methotrimeprazine
Levomepromazine
RN: 60-99-1 **MP** (°C)**:** 117
MW: 328.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.089E-05	2.000E-02	25	A081	1 0 1 1 0	EFG

4029. $C_{19}H_{24}N_2O_2$
Praziquantel
2-Cyclohexyl-carbonyl-1,3,4,6,7,11b-hexahydro-2H-pyrazine(2,1-a)isoquinoline-4-one
Biltricide
Droncit
RN: 55268-74-1 **MP** (°C)**:**
MW: 312.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.812E-01	30	B402	2 0 1 1 0	EFG
1.280E-03	4.000E-01	ns	K444	0 0 0 0 0	

4030. $C_{19}H_{24}N_2O_2S$
Cyclohexyl-*p*-toluene sulfonamide
Cyclohexyl-4-toluene sulfonamide
RN: **MP** (°C)**:**
MW: 344.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-04	6.000E-02	ns	F014	0 0 0 0 0	

4031. $C_{19}H_{24}N_4O_7$
Propyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 420.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	1.387E-01	25	M316	1 1 1 1 2	

4032. $C_{19}H_{24}O$
1,1-Dimethyl-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane
RN: 56265-26-0 **MP** (°C)**:**
MW: 268.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-07	1.800E-04	rt	C122	0 0 0 0 0	

4033. $C_{19}H_{24}O_2$
1,1,1-Trimethyl-2,2-bis(*p*-methyloxylphenyl)ethane
RN: 4741-74-6 **MP** (°C)**:**
MW: 284.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.426E-06	6.900E-04	rt	C122	0 0 0 0 0	

4034. $C_{19}H_{24}O_3$
Adrenosterone
Androstene-3,11,17-trione
RN: 382-45-6 **MP** (°C)**:** 220
MW: 300.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.279E-04	9.849E-02	23.5	J003	2 0 2 1 2	average of 2
2.610E-04	7.840E-02	37	H004	0 0 0 0 0	
5.059E-04	1.520E-01	37	J003	1 0 2 1 2	

4035. $C_{19}H_{25}NO$

N,*N*-Dicyclopentylcinnamamide

2-Propenamide, *N*,*N*-dicyclopentyl-3-phenyl-

RN: 59832-08-5 **MP** (°C)**:**

MW: 283.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-07	2.196E-04	ns	H350	0 0 0 0 0	

4036. $C_{19}H_{26}I_3N_3O_{10}$

1,3-Benzenedicarboxamide, *N*,*N′*-bis[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-

RN: 77868-46-3 **MP** (°C)**:**

MW: 837.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-02	1.961E+01	25	P091	0 0 0 0 0	

4037. $C_{19}H_{26}N_6O_4S$

Benzenesulfonamide, 4-(1,3-diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-*N*-[2-(dimethylamino)ethyl]-

RN: 89073-49-4 **MP** (°C)**:** 264

MW: 434.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-04	1.100E-01	ns	H316	0 0 0 0 0	pH 7.4
2.647E-02	1.150E+01	ns	H316	0 0 0 0 0	0.1N HCL

4038. $C_{19}H_{26}O$

δ-4-Androstene-3-one

RN: **MP** (°C)**:**

MW: 270.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-06	<2.70E-04	25	E014	2 2 2 1 0	pH 7.3

4039. $C_{19}H_{26}O_2$
Androstenedione
4-Androstene-3,17-dione
Androst-4-en-3,17-dion
RN: 63-05-8 **MP** (°C)**:**
MW: 286.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.728E-02	25	E014	2 2 2 1 2	pH 7.3
2.840E-02	8.133E+00	25	P324	0 0 0 0 0	
1.399E-04	4.007E-02	37	H034	1 0 2 1 2	pH 7.4
1.700E-04	4.870E-02	37	L010	2 0 2 1 1	

4040. $C_{19}H_{27}N_3O$
Doxylamine ethanamine
RN: **MP** (°C)**:**
MW: 313.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	9.403E+00	37.5	L034	2 2 0 1 2	pH 7.4

4041. $C_{19}H_{27}N_3O_2$
2-Propoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-propoxyquinoline-4-carboxamide
RN: 2717-00-2 **MP** (°C)**:**
MW: 329.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-04	1.311E-01	ns	B018	0 0 0 0 2	
3.980E-04	1.311E-01	ns	M066	0 0 0 0 2	

4042. $C_{19}H_{28}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-undecyl ester
RN: 65267-95-0 **MP** (°C)**:**
MW: 375.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-05	7.420E-03	ns	M120	0 0 1 1 2	

4043. $C_{19}H_{28}N_4O_6$
2′-Octanyl-6-methoxypurine arabinoside
RN: 145913-41-3 **MP** (°C)**:** 75–77
MW: 408.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.110E-04	2.496E-01	37	C348	0 0 0 0 0	pH 7.00

4044. $C_{19}H_{28}O$
7α-Methyl-19-nortestosterone
Trestolone
19-Nor-7α-methyltestosterone
RN: 3764-87-2 **MP** (°C)**:**
MW: 272.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-04	9.200E-02	37	H004	0 0 0 0 0	

4045. $C_{19}H_{28}O_2$
Androstanedione
5α-Androstane-3,17-dione
RN: 846-46-8 **MP** (°C)**:** 142
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-04	3.290E-02	23.5	J003	1 0 2 1 2	average of 2
2.200E-04	6.346E-02	25	E014	2 2 2 1 2	pH 7.3
1.685E-04	4.860E-02	37	J003	1 0 2 1 2	average of 2

4046. $C_{19}H_{28}O_2$
Testosterone
17β-Hydroxyandrost-4-en-3-one
Halotensin
Virilon
Oreton
Testex
RN: 58-22-0 **MP** (°C)**:** 155
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-05	1.615E-02	10	B012	2 0 1 1 0	
6.390E-05	1.843E-02	10	L017	2 2 2 2 2	
2.254E-04	6.500E-02	15	F042	2 2 2 2 1	
7.550E-05	2.178E-02	15	L017	2 2 2 2 2	
7.900E-05	2.279E-02	20	B012	2 0 1 1 0	

(*continued*)

4046. $C_{19}H_{28}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.430E-04	7.009E-02	20	F012	1 0 1 1 1	
2.392E-04	6.900E-02	20	F042	2 2 2 2 1	
8.460E-05	2.440E-02	20	G072	1 2 2 1 2	
7.790E-05	2.247E-02	20	L017	2 2 2 2 2	
8.000E-05	2.307E-02	20	L070	1 2 0 2 0	EFG
6.870E-05	1.982E-02	20	L077	1 2 2 2 2	
8.000E-04	2.307E-01	20	L087	1 1 2 1 0	EFG
6.240E-05	1.800E-02	22.5	B422	2 0 2 2 2	
8.100E-05	2.336E-02	25	B012	2 0 1 1 0	
9.500E-05	2.740E-02	25	B041	1 0 2 2 1	
2.531E-04	7.300E-02	25	F042	2 2 2 2 1	
8.321E-05	2.400E-02	25	K003	2 1 1 1 1	
1.664E-04	4.800E-02	25	L009	1 0 0 1 1	
8.480E-05	2.446E-02	25	L017	2 2 2 2 2	
6.934E-05	2.000E-02	25	L338	1 0 1 1 2	
1.040E-04	3.000E-02	27.34	L077	1 2 2 2 2	
1.060E-04	3.057E-02	30	B012	2 0 1 1 0	
2.670E-04	7.700E-02	30	F042	2 2 2 2 1	
9.790E-05	2.824E-02	30	L017	2 2 2 2 2	
1.100E-04	3.173E-02	30	L068	1 0 0 1 0	EFG
2.500E-04	7.211E-02	30	L344	2 0 1 1 0	
1.040E-04	3.000E-02	30	M007	2 2 1 2 2	average of 8
8.876E-05	2.560E-02	30	T005	2 0 2 2 2	
1.096E-04	3.163E-02	31	A025	2 2 2 2 0	EFG
1.300E-04	3.750E-02	35	L017	2 2 2 2 2	
1.397E-04	4.029E-02	35	L077	1 2 2 2 2	
1.950E-04	5.624E-02	37	B013	1 0 2 2 0	average
1.250E-04	3.605E-02	37	E014	2 2 2 1 2	pH 7.3
1.013E-04	2.922E-02	37	H034	1 0 2 1 2	pH 7.4
1.259E-04	3.631E-02	37.50	B041	1 0 2 2 0	EFG
1.260E-04	3.634E-02	37.50	B041	1 0 2 2 2	
1.400E-04	4.038E-02	40	B012	2 0 1 1 0	
1.570E-04	4.528E-02	40	L017	2 2 2 2 2	
3.000E-04	8.653E-02	40	L070	1 2 0 2 0	EFG
1.702E-04	4.909E-02	42.34	L077	1 2 2 2 2	
1.870E-04	5.394E-02	45	L017	2 2 2 2 2	
2.100E-04	6.057E-02	50	B012	2 0 1 1 0	
2.350E-04	6.778E-02	50	L017	2 2 2 2 2	
2.053E-04	5.922E-02	50	L077	1 2 2 2 2	
6.795E-05	1.960E-02	ns	B057	0 2 1 1 2	
3.814E-05	1.100E-02	ns	B338	0 0 0 0 1	

4047. $C_{19}H_{28}O_2$
5,6-Dehydroisoandrosterone
Prasterone
Dehydroepiandrosterone
Dehydroisoandrosterone
RN: 53-43-0 **MP** (°C)**:** 140.5
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.558E-05	2.180E-02	23.5	J003	2 0 2 1 2	average of 6
1.000E-04	2.884E-02	37	E014	2 2 2 1 2	pH 7.3
1.040E-04	3.000E-02	37	H034	1 0 2 1 2	pH 7.4
1.144E-04	3.300E-02	37	J003	1 0 2 1 2	average of 4
8.633E-05	2.490E-02	ns	B057	0 2 1 1 2	

4048. $C_{19}H_{28}O_2.H_2O$
Testosterone (monohydrate)
Testosterone monohydrate -I
RN: 58-22-0 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.920E-02	15	F042	2 2 2 2 2	crystal-II
5.352E-05	1.640E-02	15	F042	2 2 2 2 2	crystal-I
7.081E-05	2.170E-02	20	F042	2 2 2 2 2	crystal-II
6.265E-05	1.920E-02	20	F042	2 2 2 2 2	crystal-I
8.256E-05	2.530E-02	25	F042	2 2 2 2 2	crystal-II
7.310E-05	2.240E-02	25	F042	2 2 2 2 2	crystal-I
9.333E-05	2.860E-02	30	F042	2 2 2 2 2	crystal-II
8.484E-05	2.600E-02	30	F042	2 2 2 2 2	crystal-I

4049. $C_{19}H_{28}O_3$
11-Ketoetiocholanolone
3α-Hydroxy-5β-androstane-11,17-dione
Etiocholanol-11-one
Ba 2684
RN: 739-27-5 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.269E-01	23	J003	2 0 2 1 2	average of 4
9.457E-04	2.879E-01	37	J003	1 0 2 1 2	average of 2

4050. $C_{19}H_{29}ClN_5O_6$
Terazosin
Hytrin
1-(4-Amino-6,7-dimethoxy-2-quinazolinyl)-4-((tetra-hydro-2-furanyl)carbonyl)-, monohydrochloride, dihydrate
(*RS*)-Piperazine
RN: 63590-64-7 **MP** (°C)**:**
MW: 458.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-05	3.060E-02	22.5	B440	0 0 0 0 0	

4051. $C_{19}H_{29}NO$
n-Decylcinnamamide
2-Propenamide, *N*-decyl-3-phenyl-
RN: 59832-02-9 **MP** (°C)**:**
MW: 287.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-06	7.272E-04	ns	H350	0 0 0 0 0	

4052. $C_{19}H_{29}NO$
Procyclidine
Kemadrin
RN: 77-37-2 **MP** (°C)**:**
MW: 287.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.669E-06	1.055E-03	22.5	B440	0 0 0 0 0	

4053. $C_{19}H_{29}N_5O_6$
9-(1,3-Dipivaloate-2-propoxymethyl)guanine
RN: 88110-72-9 **MP** (°C)**:** 231
MW: 423.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-05	7.000E-03	25	B360	0 0 0 0 0	

4054. $C_{19}H_{30}O$
Androstane-17-one
RN: 36378-49-1 **MP** (°C)**:** 119
MW: 274.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-07	<5.49E-05	25	E014	2 2 2 1 0	pH 7.3

4055. $C_{19}H_{30}OS$
Epitiostanol
RN: 2363-58-8 **MP** (°C)**:** 127
MW: 306.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.915E-06	1.200E-03	37	H120	1 1 1 1 1	normal saline

4056. $C_{19}H_{30}O_2$
Epiandrosterone
Isoandrosterone
RN: 481-29-8 **MP** (°C)**:** 161
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.955E-05	2.020E-02	23.5	J003	2 0 2 1 2	average of 5
8.160E-05	2.370E-02	37	J003	1 0 2 1 2	average of 3

4057. $C_{19}H_{30}O_2$
Androsterone
3α-Hydroxy-17-androstanone
3α-Hydroxy-5α-androstan-17-one
Hydroxy-5α-androstan-17-one
Epihydroxyetioallocholan-17-one
Hydroxy-17-androstanone
RN: 53-41-8 **MP** (°C)**:** 185
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-05	1.150E-02	23.5	J003	2 0 2 1 2	average of 2
4.300E-05	1.249E-02	37	E014	2 2 2 1 1	pH 7.3
6.163E-05	1.790E-02	37	J003	1 0 2 1 2	average of 2

4058. $C_{19}H_{30}O_2$
Stanolone
Androstanolone
RN: 521-18-6 **MP** (°C)**:** 181.0
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.185E+00	3.443E+02	ns	B057	0 2 1 1 2	

4059. $C_{19}H_{30}O_2$
Etiocholanolone
3α-Hydroxy-5β-androstane-17-one
5-Isoandrosterone
RN: 53-42-9 **MP** (°C)**:**
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.002E-04	2.910E-02	23.5	J003	2 0 2 1 2	average of 2
7.000E-05	2.033E-02	25	E014	2 2 2 1 1	pH 7.3, pyrogen

4060. $C_{19}H_{30}O_3$
p-(Dodecyloxy)benzoic acid
Dodecyl *p*-hydroxybenzoate
RN: 2312-15-4 **MP** (°C)**:** 95
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E-03	1.094E+00	25	D081	1 2 2 1 2	

4061. $C_{19}H_{30}O_3$
Androstane-3-β,11-β-diol-17-one
Hydroxyisoandrosterone
RN: 514-17-0 **MP** (°C)**:** 235
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.552E-04	7.819E-02	23.5	J003	1 0 2 1 2	average of 2

4062. $C_{19}H_{30}O_3$
11-Hydroxyetiocholanolone
5β-Androstan-17-one, 3α,11-dihydroxy-
RN: 3272-49-9 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	4.290E-02	23.5	J003	2 0 1 1 2	average of 2

4063. $C_{19}H_{31}NO_2$
Dodecyl *p*-aminobenzoate
p-Aminobenzoic acid dodecyl ester
RN: 20043-94-1 **MP** (°C)**:**
MW: 305.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-08	4.887E-06	37	F006	1 1 2 2 1	

4064. $C_{19}H_{31}NO_3$
4-Hexoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-74-9 **MP** (°C)**:**
MW: 321.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.286E-02	ns	M066	0 0 0 0 1	

4065. $C_{19}H_{31}NO_9$
Metoprolol tartrate
1-(Isopropylamino)-3-(*p*-(2-methoxyethyl)phenoxy)-2-propanol (2:1)
RN: 56392-17-7 **MP** (°C)**:**
MW: 417.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-01	4.300E+01	25	A412	1 0 2 2 1	int

4066. $C_{19}H_{32}$
2-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4067. $C_{19}H_{32}$
6-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4068. $C_{19}H_{32}$
5-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4069. $C_{19}H_{32}$
4-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4070. $C_{19}H_{32}$
3-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4071. $C_{19}H_{32}N_2O_2$
4-Hexylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-57-6 **MP** (°C)**:**
MW: 320.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	6.089E-02	ns	M066	0 0 0 0 1	

4072. $C_{19}H_{32}O_3$
4-Nonylphenol diethoxylate
RN: 20427-84-3 **MP** (°C)**:**
MW: 308.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-05	3.640E-03	2	A335	0 0 0 0 0	
1.080E-05	3.331E-03	10	A335	0 0 0 0 0	
1.096E-05	3.380E-03	10	A335	0 0 0 0 0	
9.700E-06	2.992E-03	14	A335	0 0 0 0 0	
9.726E-06	3.000E-03	14	A335	0 0 0 0 0	
1.100E-05	3.393E-03	20.5	A335	0 0 0 0 0	
1.096E-05	3.380E-03	20.5	A335	0 0 0 0 0	
1.200E-05	3.702E-03	25	A335	0 0 0 0 0	
1.196E-05	3.690E-03	25	A335	0 0 0 0 0	

4073. $C_{19}H_{34}O_3$
Methoprene
Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate
Kabat
Precor
Dianex
Pharorid
RN: 40596-69-8 **MP** (°C)**:** 164
MW: 310.48 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.477E-06	1.390E-03	25	D302	1 0 0 0 2	
6.442E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG

4074. $C_{19}H_{40}$
2,6,10,14-Tetramethylpentadecane
Pristane
RN: 1921-70-6 **MP** (°C)**:**
MW: 268.53 **BP** (°C)**:** 296

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.724E-11	1.000E-08	25	T423	0 0 0 0 0	

4075. $C_{20}H_9Cl_3F_5N_3O_3$

Chlorfluazuron
Atabron
Benzamide, *N*-[4-(3-chloro-5-trifluoromethyl-2-pyridinyl-oxy)-3,5-dichloro-phenyl-aminocarbonyl]-2,6-difluoro
Jupiter

RN: 71422-67-8 **MP** (°C)**:**
MW: 540.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-09	1.200E-06	20	M402	0 0 0 0 0	

4076. $C_{20}H_{12}$

Benzo(a)pyrene
1,2-Benzopyrene
3,4-Benzpyrene
Benzo[a]pyrene
Benz[a]pyrene

RN: 50-32-8 **MP** (°C)**:** 179
MW: 252.32 **BP** (°C)**:** 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.309E-09	8.350E-07	15	B385	0 0 0 0 0	
2.000E-09	5.046E-07	20	E009	1 0 0 0 1	
2.972E-05	7.500E-03	23	T025	1 2 0 1 1	*sic*
6.341E-09	1.600E-06	25	B319	2 0 1 2 1	
5.667E-09	1.430E-06	25	B385	0 0 0 0 0	
7.213E-09	1.820E-06	25	D406	1 2 2 2 2	
4.400E-10	1.110E-07	25	K123	1 0 2 2 1	
1.506E-08	3.800E-06	25	L332	1 1 1 1 2	
1.506E-08	3.800E-06	25	M064	1 1 2 2 1	
1.500E-08	3.785E-06	25	M342	1 0 1 1 1	
6.428E-09	1.622E-06	25.04	M183	1 2 1 1 2	
1.585E-08	4.000E-06	27	D003	1 0 0 1 1	
9.083E-09	2.292E-06	30.04	M183	1 2 1 1 2	
1.098E-08	2.770E-06	35	B385	0 0 0 0 0	
1.506E-08	3.800E-06	ns	M344	0 0 0 0 2	
2.400E-08	6.056E-06	ns	W005	0 0 1 2 1	
4.756E-09	1.200E-06	ns	W302	0 0 0 0 1	

4077. $C_{20}H_{12}$
Benzo(k)fluoranthene
11,12-Benzo[k]fluoranthene
11,12-Benzofluoranthene
8,9-Benzofluoranthene
2,3,1′,8′-Binaphthylene
B[K]F
RN: 207-08-9 **MP** (°C)**:** 216
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-09	1.090E-06	25	D406	1 2 2 2 2	
3.171E-09	8.000E-07	ns	W302	0 0 0 0 0	

4078. $C_{20}H_{12}$
Benzo(j)fluoranthene
Benzo[l]fluoranthene
Benzo-12,13-fluoranthene
10,11-Benzofluoranthene
RN: 205-82-3 **MP** (°C)**:** 165
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.908E-09	2.500E-06	ns	W302	0 0 0 0 1	

4079. $C_{20}H_{12}$
Benzo(e)pyrene
4,5-Benzopyrene
B[E]P
RN: 192-97-2 **MP** (°C)**:** 178.5
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-09	9.840E-07	25	K123	1 0 2 2 1	
~1.59E-08	~4.00E-06	25	S227	1 2 1 1 0	
6.625E-02	1.672E+01	318	S355	1 1 1 2 0	EFG
1.192E-01	3.007E+01	330	S355	1 1 1 2 0	EFG
1.524E-01	3.846E+01	335	S355	1 1 1 2 0	EFG
2.066E-01	5.213E+01	342	S355	1 1 1 2 0	EFG
4.246E-01	1.071E+02	361	S355	1 1 1 2 0	EFG
4.559E-01	1.150E+02	365	S355	1 1 1 2 0	EFG

4080. $C_{20}H_{12}$
Perylene
Dibenz[de,kl]anthracene
peri-Dinaphthalene
RN: 198-55-0 **MP** (°C)**:** 273
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-10	1.060E-07	20	E009	1 0 0 1 1	
1.585E-09	4.000E-07	25	M064	1 1 2 2 0	
1.600E-09	4.037E-07	25	M342	1 0 1 1 1	
<1.98E-09	<5.00E-07	27	D003	1 0 0 1 0	
1.585E-09	4.000E-07	ns	M344	0 0 0 0 1	

4081. $C_{20}H_{12}$
Benzo(b)fluoranthene
3,4-Benzofluoranthene
2,3-Benzofluoranthene
B[B]F
RN: 205-99-2 **MP** (°C)**:** 108
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.945E-09	1.500E-06	ns	W302	0 0 0 0 1	

4082. $C_{20}H_{13}N$
13H-Dibenzo(a,i)carbazole
1:2,7:8-Dibenzocarbazole
RN: 239-64-5 **MP** (°C)**:** 220
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.00E-08	<1.34E-05	22	B175	1 0 1 1 0	*sic*
3.890E-08	1.040E-05	24	H106	1 0 2 2 2	
3.890E-08	1.040E-05	24	M303	1 0 1 1 2	

4083. $C_{20}H_{13}N$
3,4,5,6-Dibenzocarbazole
3:4,5:6-Dibenzocarbazole
RN: 194-59-2 **MP** (°C)**:** 158
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-07	5.347E-05	22	B175	1 0 1 1 0	

4084. $C_{20}H_{13}N$
1,2,5,6-Dibenzocarbazole
1:2,5:6-Dibenzocarbazole
RN: 207-84-1 **MP** (°C)**:**
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.337E-05	22	B175	1 0 1 1 0	

4085. $C_{20}H_{14}$
3,4′-Ace-1,2-benzanthracene
Benz[k]acephenanthrene
RN: 5779-79-3 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-08	2.700E-06	27	D003	1 0 0 1 1	

4086. $C_{20}H_{14}$
Cholanthrene
1,2-Dihydroxybenz[j]aceanthrylene
RN: 479-23-2 **MP** (°C)**:** 173
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.376E-08	3.500E-06	27	D003	1 0 0 1 1	

4087. $C_{20}H_{14}I_6N_2O_6$
Di(3-carboxy-2,4,6-triiodoanilido)adipic acid
Iodipamide
RN: 606-17-7 **MP** (°C)**:** 306
MW: 1139.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-04	4.600E-01	20	N035	1 1 2 1 1	
>4.38E-04	>5.00E-01	ns	B404	0 2 1 1 0	
1.404E-04	1.600E-01	ns	H055	0 0 0 0 0	

4088. $C_{20}H_{14}N_2O_2$
Disperse blue 19
C.I. Disperse blue 19
RN: 4395-65-7 **MP** (°C)**:** 194
MW: 314.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-10	1.918E-07	25	B333	0 0 0 0 0	
2.100E-07	6.601E-05	60.0	D093	1 2 1 2 0	EFG
5.000E-07	1.572E-04	71.8	D093	1 2 1 2 0	EFG
1.700E-06	5.344E-04	81.4	D093	1 2 1 2 0	EFG
4.200E-06	1.320E-03	97.4	D093	1 2 1 2 0	EFG

4089. $C_{20}H_{14}O_2$
3,3-Diphenylphthalide
3,3-Diphenyl-phthalid
RN: 596-29-2 **MP** (°C)**:**
MW: 286.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	4.000E-02	25	F300	1 0 0 0 0	

4090. $C_{20}H_{14}O_4$
Phenolphthalein
2-[bis(4-Hydroxyphenyl)methyl]benzoic acid
Espotabs
Alophen
Figsen
Laxettes
RN: 77-09-8 **MP** (°C)**:** 260.0
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.000E-03	25	H064	1 2 2 0 2	
7.476E-04	2.380E-01	100	H064	1 2 2 0 2	
1.256E-03	3.998E-01	rt	D021	0 0 1 1 0	

4091. $C_{20}H_{14}O_4$
Phenyl phthalate
Diphenyl phthalate
RN: 84-62-8 **MP** (°C)**:** 71
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.576E-07	8.200E-05	24	H116	2 1 0 0 1	

4092. $C_{20}H_{14}O_4$
Diphenyl *o*-phthalate
RN: **MP** (°C)**:** 72 C
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.424E-06	3.000E-03	25	S417	0 0 0 0 0	

4093. $C_{20}H_{15}O_5P$
bis(4-Carboxyphenyl)phenylphosphine oxide
BCPPO
RN: 803-19-0 **MP** (°C)**:**
MW: 366.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	7.326E-02	23	W402	0 0 0 0 0	
3.166E-04	1.160E-01	32	W402	0 0 0 0 0	
4.666E-04	1.709E-01	40	W402	0 0 0 0 0	
6.943E-04	2.543E-01	50	W402	0 0 0 0 0	
1.011E-03	3.702E-01	60	W402	0 0 0 0 0	
1.638E-03	6.000E-01	70	W402	0 0 0 0 0	
1.987E-03	7.280E-01	75	W402	0 0 0 0 0	

4094. $C_{20}H_{16}$
5,6-Dimethylchrysene
Chrysene, 5,6-dimethyl-
RN: 3697-27-6 **MP** (°C)**:** 127
MW: 256.35 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.752E-08	2.500E-05	27	D003	1 0 0 1 1	

4095. $C_{20}H_{16}$
9,10-Dimethyl-1,2-benzanthracene
7,12-Dimethyl-1,2-benzanthracene
7,12-Dimethylbenz[a]anthracene
9,10-Dimethyl-benz[a]anthracene
RN: 56-56-4 **MP** (°C)**:** 122
MW: 256.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.518E-08	2.440E-05	24	H106	1 0 2 2 2	
2.145E-07	5.500E-05	24	H116	2 1 0 0 1	
9.752E-08	2.500E-05	24	M129	1 2 1 1 1	
2.380E-07	6.100E-05	25	M064	1 1 2 2 1	
9.518E-08	2.440E-05	25	M156	1 2 1 1 2	
1.677E-07	4.300E-05	27	D003	1 0 0 1 1	

4096. $C_{20}H_{16}$
10-Ethyl-1,2-benzanthracene
10-Ethylbenz[a]anthracene
RN: 14854-08-1 **MP** (°C)**:** 114
MW: 256.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.755E-07	4.500E-05	27	D003	1 0 0 1 1	
1.560E-07	4.000E-05	27	D043	2 0 0 0 0	average of 2

4097. $C_{20}H_{16}O_4$
Phenolphthalin
Benzoic acid, 2-[bis(4-hydroxyphenyl)methyl]-
RN: 81-90-3 **MP** (°C)**:** 237
MW: 320.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.463E-04	1.750E-01	20	F300	1 0 0 0 2	

4098. $C_{20}H_{17}FO_3S$
Sulindac
Aclin
Clinoril
Clusinol
Saldac
RN: 38194-50-2 **MP** (°C)**:**
MW: 356.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-05	7.000E-03	37	Y421	0 0 0 0 0	

4099. $C_{20}H_{18}O_2Sn$
Triphenyltin hydroxide acetate
Fentin acetate
RN: 900-95-8 **MP** (°C)**:** 120
MW: 409.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.845E-05	2.800E-02	20	M161	1 0 0 0 1	

4100. $C_{20}H_{18}O_{10}$
Biphenyl dimethyl dicarboxylate
DDB
RN: **MP** (°C)**:**
MW: 418.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E-05	4.200E-03	ns	K446	0 0 0 0 0	

4101. $C_{20}H_{19}NO_3$
Acronine
3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano(2,3-c)acridin-7-one
Acronycine
RN: 7008-42-6 **MP** (°C)**:** 175–176
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.779E-06	2.500E-03	22	B064	1 0 1 1 0	
8.401E-06	2.700E-03	25	R071	0 0 0 0 0	

4102. $C_{20}H_{19}NO_5.6H_2O$
Berberine (hexahydrate)
Berberine
RN: 2086-83-1 **MP** (°C)**:** 145dec
MW: 461.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.422E-02	4.348E+01	25	D004	0 0 0 0 0	

4103. $C_{20}H_{19}N_3$
Rosaniline
Basic violet 14
C.I. 42510
Calcozine magenta xx
Cerise B
RN: 632-99-5 **MP** (°C)**:**
MW: 301.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.951E-04	2.999E-01	rt	D021	0 0 1 1 0	

4104. $C_{20}H_{19}N_3O_5$

1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, propyl ester

RN: 153474-31-8 **MP** (°C)**:** 113.5
MW: 381.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5

4105. $C_{20}H_{20}ClNO_7$

BTA-243

1,3-Benzodioxole-2,2-dicarboxylic acid, 5-[2-[[2-(3-chlorophenyl)-2-hydroxyethyl]amino] propyl]-

RN: **MP** (°C)**:**
MW: 421.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.890E-03	3.750E+00	25	B421	0 0 1 1 0	Zwitterion, EFG

4106. $C_{20}H_{20}N_2O_6$

Succinyl acetaminophen

Butanedioic acid, bis[4-(acetylamino)phenyl] ester

Acetanilide, 4′-hydroxy-, succinate

Acetanilide, 4′-hydroxy-, succinate (2:1) (ester)

RN: 2725-63-5 **MP** (°C)**:** 229–230
MW: 384.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.769E-05	6.800E-03	37	D029	0 0 0 0 0	

4107. $C_{20}H_{20}N_6O_6S_2$

2,5-Di-(*N*4-acetylsulfanilylamino)pyrimidine

RN: **MP** (°C)**:**
MW: 504.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.910E-06	5.000E-03	37	R076	1 2 0 0 1	

4108. $C_{20}H_{21}ClO_4$
Fenofibrate
Proctofene
Sedufen
RN: 49562-28-9 **MP** (°C)**:**
MW: 360.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E-06	8.000E-04	25	J415	0 0 0 0 0	

4109. $C_{20}H_{21}NO_4$
Papaverine
Pantoyl taurine
RN: 58-74-2 **MP** (°C)**:** 147
MW: 339.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.733E-02	37.5	L034	2 2 0 1 2	pH 7.4

4110. $C_{20}H_{21}NO_5$
Aspirin phenylalanine ethyl ester
L-Phenylalanine, *N*-[2-(acetyloxy)benzoyl]-, ethyl ester
RN: 76748-72-6 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	1.670E-01	25	B182	2 2 1 1 1	

4111. $C_{20}H_{21}NO_5$
Repirinast
Isoamyl 5,6-dihydro-7,8-dimethyl-4,5-dioxo-4H-pyrano(3,2-c)quinoline-2-carboxylate
RN: 73080-51-0 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-06	1.200E-03	ns	S470	0 0 0 0 0	

4112. $C_{20}H_{22}ClN$
Pyrrobutamine
Pyrrolidine, 1-[4-(4-chlorophenyl)-3-phenyl-2-butenyl]-
RN: 91-82-7 **MP** (°C)**:**
MW: 311.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	2.713E-01	37.5	L034	2 2 0 1 2	pH 7.4

4113. $C_{20}H_{22}FN_3O_7$
3-Quinolinecarboxylic acid
7-[4-[[(acetyloxy)methoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-
RN: 99106-30-6 **MP** (°C)**:**
MW: 435.41 **BP** (°C)**:** 636.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.445E-04	1.500E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.378E-04	6.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
6.890E-05	3.000E-02	25	A414	1 0 1 1 1	pH 5 phosphate buffer (0.1 M)

4114. $C_{20}H_{22}N_2O_2$
Quininone
Chininon
Cinchonan-9-one, 6′-methoxy-, (8α)-
RN: 84-31-1 **MP** (°C)**:** 212
MW: 322.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.305E-06	3.000E-03	20	F300	1 0 0 0 0	

4115. $C_{20}H_{22}N_8O_5$
Methotrexate
(+)-4-Amino-10-methylfolic acid
Metatrexan
Methoblastin
Maxtrex
Ledertrexate
RN: 59-05-2 **MP** (°C)**:** 195
MW: 454.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.290E+00	1.950E+03	c	B443	0 0 0 0 0	
2.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4116. $C_{20}H_{23}N$
Maprotiline
Maprotyline
RN: 10262-69-8 **MP** (°C)**:**
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	8.334E-04	22.5	B440	0 0 0 0 0	

4117. $C_{20}H_{23}NO_2$
Dexoxadrol
(+)-2-(2,2-Diphenyl-1,3-dioxolan-4-yl)piperidine
Relane
CL 911C
RN: 4741-41-7 **MP** (°C)**:**
MW: 309.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	7.000E-02	rt	K017	0 2 2 2 2	intrinsic

4118. $C_{20}H_{23}N_7O_7$
*N*5-Formyltetrahydropteroylglutamic acid
RN: 58-05-9 **MP** (°C)**:**
MW: 473.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.85E+00	>1.35E+03	25	B443	0 0 0 0 0	

4119. $C_{20}H_{24}ClN_3S$
Prochlorperazine
Compazine
Ultrazine
Cotranzine
Compa-Z
RN: 58-38-8 **MP** (°C)**:** 228
MW: 373.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.496E-02	24	G022	2 0 1 1 1	

4120. $C_{20}H_{24}N_2$
Dimethindene
Dimetindene
Pyridine, 2-[1-[2-[2-(dimethylamino)ethyl]inden-3-yl]ethyl]-
RN: 5636-83-9 **MP** (°C)**:**
MW: 292.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.160E-04	2.386E-01	37	L094	2 0 0 1 2	pH>10.03, intrinsic

4121. $C_{20}H_{24}N_2O_2$
Quinine
Chinin
Quinine alkaloid
RN: 130-95-0 **MP** (°C)**:** 177
MW: 324.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E-03	5.000E-01	15	F300	1 0 0 0 0	
9.555E-05	3.100E-02	22	M459	0 0 0 0 0	
1.760E-03	5.711E-01	25	D004	0 0 0 0 0	
9.247E-04	3.000E-01	25	P015	0 0 0 0 0	
4.007E-03	1.300E+00	100	F300	1 0 0 0 1	
<3.08E-04	<1.00E-01	rt	B435	0 0 0 0 0	
1.756E-03	5.697E-01	rt	D021	0 0 1 1 1	

4122. $C_{20}H_{24}N_2O_2$
Quinidine
Chinidin
Cinchonan-9-ol, 6′-methoxy-, (9*S*)-
RN: 56-54-2 **MP** (°C)**:** 174
MW: 324.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	2.336E-01	15	K059	2 2 2 0 1	
1.110E-04	3.600E-02	22	M459	0 0 0 0 0	
4.315E-04	1.400E-01	25	F300	1 0 0 0 1	
1.540E-03	4.998E-01	c	D004	0 0 0 0 0	
3.848E-03	1.248E+00	h	D004	0 0 0 0 0	
1.549E-03	5.025E-01	ns	R427	0 0 0 0 0	

4123. $C_{20}H_{24}N_2O_2.3H_2O$
Quinine (trihydrate)
Quinine, compd. with valeric acid (1:1), hydrate
Cinchonan-9-ol, 6′-methoxy-, trihydrate, (8α,9*R*)-
RN: 6151-51-5 **MP** (°C)**:** 57
MW: 378.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-03	6.406E-01	c	D004	0 0 0 0 0	
3.299E-03	1.248E+00	h	D004	0 0 0 0 0	

4124. $C_{20}H_{24}N_2O_4$
Pheniramine maleate
1-Phenyl-1-(2-pyridyl)-3-dimethylaminopropane maleate
Prophenpyridamine maleate
RN: 132-20-7 **MP** (°C)**:**
MW: 356.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	1.105E+01	37.5	L034	2 2 0 1 2	pH 7.4

4125. $C_{20}H_{24}N_2O_5$
Naproxen, *N*-methyl-*N*-carbamoyl methyl-glycolamide ester
RN: **MP** (°C)**:** 179.5
MW: 372.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E-04	5.900E-02	21	B331	1 2 2 1 1	pH 7.4

4126. $C_{20}H_{24}O_3$
Methylsecodione
RN: 80702-24-5 **MP** (°C)**:**
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-03	5.996E-01	25	P324	0 0 0 0 0	

4127. $C_{20}H_{24}O_4$

3,11-Dioxo-4,17(20)-*cis*-pregnadien-21-oic acid methyl ester
U-2726
RN: **MP** (°C)**:**
MW: 328.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	4.300E-03	ns	K029	0 0 2 1 1	

4128. $C_{20}H_{24}O_6$

Dibenzo-18-crown-6
DBC
RN: 14187-32-7 **MP** (°C)**:**
MW: 360.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.025E-05	7.300E-03	25	M127	1 2 1 1 1	
9.000E-05	3.244E-02	26	P029	0 0 0 0 0	

4129. $C_{20}H_{25}ClN_2O_2$

Quinine hydrochloride
Inchonan-9-ol, 6′-methoxy-, monohydrochloride, (8α,9*R*)-
RN: 130-89-2 **MP** (°C)**:**
MW: 360.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	5.497E-01	25	A412	1 0 2 2 1	int

4130. $C_{20}H_{25}ClO_2$

1-Chloro-1,1-dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-24-8 **MP** (°C)**:**
MW: 332.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.708E-07	1.900E-04	rt	C122	0 0 0 0 0	

4131. $C_{20}H_{25}NO_2$

Adiphenine
2-Diethylaminoethyl diphenylacetate
Tranzetil
Patrovine
SKF 962A

RN: 64-95-9 **MP** (°C)**:** 113.5
MW: 311.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	3.114E+00	30	L068	1 0 0 1 0	EFG

4132. $C_{20}H_{25}NO_4$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(diethylamino)-2-oxoethyl ester, (*S*)
Naproxen, *N*,*N*-diethyl glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(diethylamino)-2-oxoethyl ester
Naproxen *N*,*N*-diethyl glycolamide ester

RN: 106231-74-7 **MP** (°C)**:** 89
MW: 343.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-05	1.200E-02	21	B331	1 2 2 1 1	pH 7.4
3.494E-05	1.200E-02	21	B331	0 0 0 0 0	

4133. $C_{20}H_{25}NO_4$

3,11-Dioxo-4,17(20)-*cis*-pregnadien-20-oic acid methyl ester 3-oxime

RN: **MP** (°C)**:**
MW: 343.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-05	5.300E-03	ns	K029	0 0 2 1 1	

4134. $C_{20}H_{25}NO_5$

Naproxen, *N*-methyl-*N*-hydroxyethyl glycolamide ester

RN: **MP** (°C)**:** 110
MW: 359.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-04	1.400E-01	21	B331	1 2 2 1 1	pH 7.4

4135. $C_{20}H_{25}NO_6$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[bis(2-hydroxyethyl)amino]-2-oxoethyl ester
Naproxen *N*,*N*-diethanol glycolamide ester
Naproxen,*N*,*N*-dihydroxyethyl glycolamide ester
RN: 114665-20-2 **MP** (°C)**:** 113
MW: 375.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-03	4.100E-01	21	B331	1 2 2 1 1	pH 7.4
1.092E-03	4.100E-01	21	B331	0 0 0 0 0	

4136. $C_{20}H_{26}N_2$

1-(Diphenylmethyl)-4-propylpiperazine
RN: **MP** (°C)**:**
MW: 294.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.448E-04	1.899E-01	25	M438	0 0 0 0 0	

4137. $C_{20}H_{26}N_2O_2$

Ajmaline
Rauwolfine
Ajmalan-17,21-diol, (17R,21α)-
Merabitol
Raugalline
RN: 4360-12-7 **MP** (°C)**:** 159
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	3.591E-01	0	M106	2 1 1 1 0	EFG
1.300E-03	4.244E-01	15	M106	2 1 1 1 0	EFG
1.500E-03	4.897E-01	30	M106	2 1 1 1 0	EFG

4138. $C_{20}H_{26}N_2O_2$

Hydroquinine
Cinchonan-9-ol, 10,11-dihydro-6′-methoxy-, (8α,9*R*)-
10,11-Dihydroquinine
RN: 522-66-7 **MP** (°C)**:** 173.5
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.063E-04	9.999E-02	20	K059	2 2 2 0 1	
>1.53E-03	>5.00E-01	ns	B404	0 2 1 1 0	

4139. $C_{20}H_{26}O_2$
Norethindrone
Norethisterone
RN: 68-22-4 **MP** (°C)**:** 203
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-05	3.981E-03	10	L078	1 0 1 2 0	EFG
1.679E-05	5.012E-03	20	L078	1 0 1 2 0	EFG
2.360E-05	7.043E-03	25	H099	1 0 2 2 2	
1.884E-05	5.623E-03	25	L078	1 0 1 2 2	
8.377E-03	2.500E+00	25	P312	0 0 0 0 0	
2.114E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
3.610E-05	1.077E-02	37	C004	0 0 0 0 0	EFG
2.986E-05	8.912E-03	40	L078	1 0 1 2 0	EFG
4.218E-05	1.259E-02	50	L078	1 0 1 2 0	EFG
3.351E-05	1.000E-02	ns	K444	0 0 0 0 0	

4140. $C_{20}H_{26}O_2$
1,1-Dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-21-5 **MP** (°C)**:**
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-07	4.300E-05	rt	C122	0 0 0 0 0	

4141. $C_{20}H_{26}O_4$
Dicyclohexyl phthalate
1,2-Benzenedicarboxylic acid, dicyclohexyl ester
RN: 84-61-7 **MP** (°C)**:** 66
MW: 330.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E-05	4.000E-03	24	H116	2 1 0 0 2	

4142. $C_{20}H_{27}NO_5S_2$
2-(Acetyloxy)-4-[2-({5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-amino)ehtyl]phenyl acetate
RN: **MP** (°C)**:**
MW: 425.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.151E-04	4.900E-02	ns	S453	0 0 0 0 0	

4143. $C_{20}H_{27}NO_{11}$
Amygdalin
(*R*)-Amygdalin
(*R*)-Laenitrile
(*R*)-Amygdaloside
RN: 29883-15-6 **MP** (°C)**:** 223
MW: 457.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	7.800E+01	10	F300	1 0 0 0 1	
1.698E-01	7.768E+01	ns	R427	0 0 0 0 0	

4144. $C_{20}H_{27}NO_{11}.3H_2O$
Amygdalin (trihydrate)
D-(–)-Amygdalin
(*R*)-Amygdalin
RN: 29883-15-6 **MP** (°C)**:** 214–216
MW: 511.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.504E-01	7.692E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

4145. $C_{20}H_{27}O_4P$
Octyldiphenyl phosphate
Disflamoll DPO
RN: 115-88-8 **MP** (°C)**:**
MW: 362.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.863E-07	1.400E-04	24	H116	2 1 0 0 2	

4146. $C_{20}H_{28}O$
Vitamin A aldehyde
Retinal
All-*trans*-retinal
All-*trans* vitamin A aldehyde
Retinene
RN: 116-31-4 **MP** (°C)**:** 63
MW: 284.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.46E-04	<7.00E-02	25	P312	0 0 0 0 0	

4147. $C_{20}H_{28}O_2$
19-Norprogesterone
19-Norpregn-4-ene-3,20-dione
RN: 472-54-8 **MP** (°C)**:**
MW: 300.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.610E-02	37	L010	2 0 2 1 1	

4148. $C_{20}H_{28}O_2$
Retinoic acid
All-*trans* retinoic acid
3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenoic acid
β-All-*trans*-retinoic acid
RN: 302-79-4 **MP** (°C)**:** 180-181
MW: 300.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.33E-04	<7.00E-02	25	P312	0 0 0 0 0	

4149. $C_{20}H_{28}O_3$
5,6-Dehydroisoandrosterone formate
Androst-5-en-17-one, 3α-hydroxy-, formate
RN: 4589-84-8 **MP** (°C)**:**
MW: 316.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.424E-05	1.400E-02	ns	B057	0 2 1 1 2	

4150. $C_{20}H_{28}O_3$
Testosterone formate
Androst-4-en-17β-ol-3-one formate
Testosterone 17-formate
RN: 3129-42-8 **MP** (°C)**:**
MW: 316.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-05	4.395E-03	25	J004	1 0 1 1 2	
1.390E-05	4.400E-03	ns	B057	0 2 1 1 1	

4151. $C_{20}H_{29}N_3O_2$
Dibucaine
Cinchocaine
RN: 85-79-0 **MP** (°C)**:** 64
MW: 343.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-04	6.801E-02	ns	B018	0 0 0 0 2	
1.980E-04	6.801E-02	ns	M066	0 0 0 0 2	

4152. $C_{20}H_{30}N_4O_6$
2′-Nonyl-6-methoxypurine arabinoside
4-Quinolinecarboxamide, 2-butoxy-*N*-[2-(diethylamino)ethyl]-
RN: 145913-42-4 **MP** (°C)**:** 88-90
MW: 422.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-04	4.352E-02	37	C348	0 0 0 0 0	pH 7.00

4153. $C_{20}H_{30}O$
D 263
4,6-Diisopropyl-1,1-dimethyl-7-propionylindan
RN: 290294-31-4 **MP** (°C)**:** 117
MW: 286.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.491E-06	1.000E-03	ns	M061	0 0 0 0 0	

4154. $C_{20}H_{30}O$
Vitamin A
Retinol
Afaxin
α-Sterol
RN: 68-26-8 **MP** (°C)**:** 62
MW: 286.46 **BP** (°C)**:** 137–138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.49E-05	<1.00E-02	25	P312	0 0 0 0 0	

4155. $C_{20}H_{30}O_2$
Abietic acid
13-Isopropylpodocarpa-7,13-dien-15-oic acid
Sylvic acid
RN: 514-10-3 **MP** (°C)**:** 172
MW: 302.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	4.839E-02	20	B009	2 2 1 2 0	

4156. $C_{20}H_{30}O_2$
17-Methyltestosterone
17-α-Methyltestosterone
Methyltestosterone
Methyl-testosterone
RN: 58-18-4 **MP** (°C)**:** 161
MW: 302.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-04	3.720E-02	20	F012	1 0 1 1 1	
1.120E-04	3.388E-02	25	H099	1 0 2 2 2	
1.058E-04	3.200E-02	25	K003	2 1 1 1 1	
4.400E-02	1.331E+01	25	M379	1 0 1 1 0	EFG,*sic*
<5.62E-04	<1.70E-01	25	P312	0 0 0 0 0	
2.313E-03	6.995E-01	25	P324	0 0 0 0 0	
1.018E-04	3.080E-02	30	T005	2 0 2 2 2	
1.200E-04	3.630E-02	37	E014	2 2 2 1 2	pH 7.3
7.472E-05	2.260E-02	ns	B057	0 2 1 1 2	
9.918E-05	3.000E-02	rt	N302	0 2 1 2 1	

4157. $C_{20}H_{30}O_3$
Androstanolone formate
5α-Androstan-3-one, 17-hydroxy-, formate
RN: 4589-90-6 **MP** (°C)**:**
MW: 318.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-06	1.490E-03	ns	B057	0 2 1 1 2	

4158. $C_{20}H_{30}O_6$
Butyl glycol phthalate
bis(2-Butoxyethyl) phthalate
Dibutoxyethyl phthalate
bis(2-*N*-Butoxyethyl) phthalate
RN: 117-83-9 **MP** (°C)**:** 230
MW: 366.46 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.458E-05	2.000E-02	15	H069	1 0 1 1 0	
<8.18E-04	<3.00E-01	20	F070	1 0 0 0 1	

4159. $C_{20}H_{31}NO$
Trihexyphenidyl
1-Phenyl-1-cyclohexyl-3-piperidyl-1-propanol hydrochloride
Artane
Benzhexol chloride
Trihexyphenidyl-D,L hydrochloride
Tremin
RN: 52-49-3 **MP** (°C)**:**
MW: 301.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	6.709E-04	22.5	B440	0 0 0 0 0	

4160. $C_{20}H_{31}NO_3$
Acetaminophen laurate
Acetaminophen dodecanoate
RN: 54942-38-0 **MP** (°C)**:** 111
MW: 333.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E-05	6.000E-03	25	B010	1 1 1 1 0	

4161. $C_{20}H_{32}O_3$
Tridecyl *p*-hydroxybenzoate
p-Hydroxybenzoic acid tridecyl ester
RN: 69679-32-9 **MP** (°C)**:**
MW: 320.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	3.639E-01	25	D081	1 2 2 1 2	

4162. $C_{20}H_{32}O_5$
Dinoprostone
Prostaglandin E2
RN: 363-24-6 **MP** (°C)**:** 66–68
MW: 352.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.123E-03	1.101E+00	8.53	F068	0 0 2 2 0	
4.022E-03	1.418E+00	19.24	F068	0 0 2 2 0	
4.173E-03	1.471E+00	25.35	F068	0 0 2 2 0	
4.575E-03	1.613E+00	29.9	F068	0 0 2 2 0	

4163. $C_{20}H_{33}NO$
Fenpropimorph
4-(3-(4-(1,1-Dimethylethyl)phenyl)-2-methylpropyl)-2,6-dimethylmorpholine
Corbe
Mistral
RN: 67306-03-0 **MP** (°C)**:**
MW: 303.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-05	4.300E-03	ns	V414	0 0 0 0 0	

4164. $C_{20}H_{33}NO_3$
4-Heptoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-75-0 **MP** (°C)**:**
MW: 335.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.677E-02	ns	M066	0 0 0 0 1	

4165. $C_{20}H_{33}N_3O_4$
Celiprolol
RN: 56980-93-9 **MP** (°C)**:**
MW: 379.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	2.290E-02	22.5	B440	0 0 0 0 0	
6.008E-09	2.280E-06	200	M418	0 0 0 0 0	

4166. $C_{20}H_{34}$
5-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4167. $C_{20}H_{34}$
2-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4168. $C_{20}H_{34}$
4-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4169. $C_{20}H_{34}$
3-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4170. $C_{20}H_{34}$
6-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4171. $C_{20}H_{34}N_2O_2$

4-Heptylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: **MP** (°C)**:**

MW: 334.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	7.025E-02	ns	M066	0 0 0 0 1	

4172. $C_{20}H_{34}O_4$

4-Octylphenol triethoxylate

RN: 51437-91-3 **MP** (°C)**:**

MW: 338.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.436E-05	1.840E-02	20.5	A335	0 0 0 0 0	
5.440E-05	1.841E-02	20.5	A335	0 0 0 0 0	

4173. $C_{20}H_{34}O_8$

Acetyl tributyl citrate

1,2,3-Propanetricarboxylic acid

Tributyl acetylcitrate

RN: 77-90-7 **MP** (°C)**:**

MW: 402.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.224E-06	1.700E-03	25	F067	1 0 2 2 1	

4174. $C_{20}H_{36}O_4$

Dioctyl maleate

2-Butenedioic acid (Z)-

Dioctyl ester

RN: 2915-53-9 **MP** (°C)**:**

MW: 340.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E-06	6.000E-04	25	F067	1 0 2 2 2	

4175. $C_{20}H_{36}O_6$
Dicyclohexyl-18-crown-6
Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, icosahydro-
Dicyclohexano-18-crown-6
cis-Dicyclohexano-18-crown-6
RN: 16069-36-6 **MP** (°C)**:**
MW: 372.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-02	1.341E+01	26	P029	0 0 0 0 0	
2.200E-02	8.195E+00	53	P029	0 0 0 0 0	
1.000E-02	3.725E+00	82	P029	0 0 0 0 0	

4176. $C_{20}H_{40}$
1-Eicosene
n-Eicosene
RN: 3452-07-1 **MP** (°C)**:**
MW: 280.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-12	5.350E-10	23	C332	0 0 0 0 0	

4177. $C_{21}H_{11}ClF_6N_2O_3$
Flufenoxuron
RN: 101463-69-8 **MP** (°C)**:**
MW: 488.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-09	3.800E-06	20	M402	0 0 0 0 0	

4178. $C_{21}H_{13}N$
1:2,6:7-Dibenzacridine
RN: 226-92-6 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.397E-05	22	B175	1 0 1 1 0	

4179. $C_{21}H_{13}N$
1:2,8:9-Dibenzacridine
RN: 224-53-3 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-08	1.955E-05	22	B175	1 0 1 1 0	

4180. $C_{21}H_{13}N$
3:4,6:7-Dibenzacridine
RN: 226-97-1 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	6.984E-05	22	B175	1 0 1 1 1	

4181. $C_{21}H_{14}$
5-Methyl-3,4-benzpyrene
RN: 31647-36-6 **MP** (°C)**:** 216
MW: 266.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-09	8.000E-07	27	D003	1 0 0 1 0	

4182. $C_{21}H_{15}ClN_2O_4S$
1-(*p*-Chlorobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-38-4 **MP** (°C)**:**
MW: 426.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.965E-07	3.400E-04	37	F183	1 0 1 1 2	intrinsic

4183. $C_{21}H_{15}N_3O_6S$
1-(*p*-Nitrobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 21413-53-6 **MP** (°C)**:**
MW: 437.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.486E-06	6.500E-04	37	F183	1 0 1 1 2	intrinsic

4184. $C_{21}H_{16}$
3-Methylcholanthrene
1,2-Dihydro-3-methyl-benz[j]aceanthrylene
20-Methylcholanthrene
RN: 56-49-5 **MP** (°C)**:** 179
MW: 268.36 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E-08	3.230E-06	24	H106	1 0 2 2 2	
1.081E-08	2.900E-06	25	M064	1 1 2 2 1	
1.204E-08	3.230E-06	25	M156	1 2 1 1 2	
1.100E-08	2.952E-06	25	M342	1 0 1 1 1	
5.589E-09	1.500E-06	27	D003	1 0 0 1 1	
1.081E-08	2.900E-06	ns	M344	0 0 0 0 1	

4185. $C_{21}H_{16}N_2O_2$
C.I. Disperse blue 24
9,10-Anthracenedione, 1-amino-4-hydroxy-2-phenoxy-
Serilene red 2BL
Sumikaron red E-FBL
Solvent red 146
RN: 17418-58-5 **MP** (°C)**:** 151
MW: 328.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.642E-05	25	B333	0 0 0 0 0	

4186. $C_{21}H_{16}N_2O_4S$
1-Benzenesulfonyl-5,5-diphenyl-hydantoin
RN: 21413-28-5 **MP** (°C)**:**
MW: 392.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.587E-06	1.800E-03	37	F183	1 0 1 1 2	intrinsic

4187. $C_{21}H_{16}N_2O_5S$
1-(*p*-Hydroxylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-35-1 **MP** (°C)**:**
MW: 408.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.080E-06	3.300E-03	37	F183	1 0 1 1 2	intrinsic

4188. $C_{21}H_{17}N_3O_2S_2$
2-Sulfanilamido-4-*p*-diphenylthiazole
RN: **MP** (°C)**:**
MW: 407.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-06	1.000E-03	37	R045	1 2 1 1 0	

4189. $C_{21}H_{17}N_3O_4S$
1-(*p*-Aminobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-34-0 **MP** (°C)**:**
MW: 407.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.436E-06	1.400E-03	37	F183	1 0 1 1 2	intrinsic

4190. $C_{21}H_{19}NO_4$
Cinmetacin
1-Cinnamoyl-2-methyl-5-methoxyindolyl-3-acetic acid
Indolacin
RN: 20168-99-4 **MP** (°C)**:** 170
MW: 349.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.86E-06	<1.00E-03	25	K027	2 0 2 2 0	

4191. $C_{21}H_{20}Cl_2O_3$
Permethrin
3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl Ester
Ambush
Pounce
Ectiban
RN: 52645-53-1 **MP** (°C)**:** 36.5
MW: 391.30 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.111E-07	2.000E-04	ns	M161	0 0 0 0 0	
~5.11E-07	~2.00E-04	ns	Y418	0 0 0 0 0	

4192. $C_{21}H_{20}O_9$
Puerarin
8-ß-D-Glucopyransyl-7-hydroxy-3-(4-hydroxyphenyl)-4H-1benzopyran-4-one
RN: 3681-99-0 **MP** (°C)**:**
MW: 416.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-01	3.373E+02	15.0	W418	0 0 0 0 0	
9.500E-01	3.956E+02	20.0	W418	0 0 0 0 0	
1.100E+00	4.580E+02	25.0	W418	0 0 0 0 0	
1.260E+00	5.246E+02	30.0	W418	0 0 0 0 0	
1.420E+00	5.913E+02	35.0	W418	0 0 0 0 0	
1.710E+00	7.120E+02	40.0	W418	0 0 0 0 0	
2.020E+00	8.411E+02	45.0	W418	0 0 0 0 0	
2.430E+00	1.012E+03	50.0	W418	0 0 0 0 0	
2.840E+00	1.183E+03	55.0	W418	0 0 0 0 0	

4193. $C_{21}H_{21}ClN_2O_8$

Demeclocycline
Declomycin
Methylchlorotetracycline
Demethylchlortetracycline

RN: 127-33-3 **MP** (°C)**:**
MW: 464.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-03	1.515E+00	21	M044	2 0 2 2 2	
3.012E-03	1.400E+00	25	B191	1 0 0 0 1	neutral pH

4194. $C_{21}H_{21}N$

Cyproheptadine

RN: 129-03-3 **MP** (°C)**:**
MW: 287.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	3.176E-04	22.5	B440	0 0 0 0 0	

4195. $C_{21}H_{21}NO_6$

Rhoeadine
[1,3]Dioxolo[4,5-h]-1,3-dioxolo[7,8][2]benzopyrano[3,4-a][3]benzazepine, 5β,6,7,8,13β,15-hexahydro-15-methoxy-6-methyl-, (5b*R*,13b*R*,15*S*)
8-Methoxy-16-methyl-2,3:10,11-bis[methylenebis(oxy)]-, (8β)-

RN: 2718-25-4 **MP** (°C)**:** 245–247dec
MW: 383.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.172E-03	8.326E-01	25	D004	0 0 0 0 0	

4196. $C_{21}H_{21}NO_6$

Hydrastine
Hydrastin
(1*R*,9*S*)-β-Hydrastine

RN: 118-08-1 **MP** (°C)**:** 132
MW: 383.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-04	3.144E-01	15	K059	2 2 2 0 1	
7.825E-05	3.000E-02	20	F300	1 0 0 0 1	

4197. $C_{21}H_{21}N_3O_3S$
L-Phe-dapsone
Benzenepropanamide, α-amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-
RN: 160349-01-9 **MP** (°C)**:**
MW: 395.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.057E-06	2.000E-03	25	P351	0 0 0 0 0	pH 7.4
3.287E-03	1.300E+00	25	P351	0 0 0 0 0	

4198. $C_{21}H_{21}O_4P$
Tricresyl phosphate
Tritolyl phosphate
Tri-*p*-cresyl phosphate
RN: 1330-78-5 **MP** (°C)**:**
MW: 368.37 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.009E-07	7.400E-05	24	H116	2 1 0 0 1	
2.715E-07	1.000E-04	25	F067	1 0 2 2 1	
2.172E-04	7.999E-02	ns	F014	0 0 0 0 0	

4199. $C_{21}H_{22}N_2O_2$
Strychnine
Strychnidin-10-one
Gopher Getter
L-Strychnine
Gopher Bait
RN: 57-24-9 **MP** (°C)**:** 275
MW: 334.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	9.029E-02	15	K059	2 2 2 0 1	
4.186E-04	1.400E-01	20.0	N002	2 1 2 2 1	
5.980E-04	2.000E-01	30.0	N002	2 1 2 2 1	
1.017E-03	3.400E-01	40.0	N002	2 1 2 2 1	
1.196E-03	4.000E-01	50.0	N002	2 1 2 2 1	
1.346E-03	4.500E-01	60.0	N002	2 1 2 2 1	
1.794E-03	6.000E-01	75.0	N002	2 1 2 2 1	
4.672E-04	1.562E-01	c	D004	0 0 0 0 0	
9.643E-04	3.225E-01	h	D004	0 0 0 0 0	
4.276E-04	1.430E-01	rt	M161	0 0 0 0 2	

4200. $C_{21}H_{22}N_2O_5$

Benzeneacetic acid, 4-benzoyl-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

N-Methyl-*N*-carbamoyl methyl glycolamide salicylate

RN: 114665-16-6 **MP** (°C)**:** 83

MW: 382.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	0 0 0 0 0	

4201. $C_{21}H_{22}N_2O_5$

Ketoprofen, *N*-methyl-*N*-carbamoylmethyl glycolamide ester

Benzeneacetic acid, 3-benzoyl-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

RN: 116482-84-9 **MP** (°C)**:** 83.5

MW: 382.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	1 2 2 1 1	pH 7.4

4202. $C_{21}H_{23}ClFNO_2$

Haloperidol

Haldol

4-[4-(*p*-Chlorophenyl)-4-hydroxypiperidino]-4′-fluorobutyrophenone

Serenace

RN: 52-86-8 **MP** (°C)**:** 148

MW: 375.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.623E-04	6.100E-02	22	J420	0 0 0 0 0	pH6.5
5.474E-06	2.058E-03	22.5	B440	0 0 0 0 0	
7.981E-06	3.000E-03	30	P044	0 0 0 0 0	
2.660E-05	1.000E-02	ns	K444	0 0 0 0 0	
<2.66E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4203. $C_{21}H_{23}N_3OS$

Pericyazine

2-Cyano-10-[3′-(4″-hydroxypiperidino)propyl]phenothiazine

Periciazine

RN: 2622-26-6 **MP** (°C)**:** 116

MW: 365.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.801E-02	37	F011	1 0 1 1 2	pH 7.4

4204. $C_{21}H_{24}FN_3O_7$
3-Quinolinecarboxylic acid
7-[4-[[1-(Acetyloxy)ethoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-
RN: 99106-35-1 **MP** (°C)**:** 216
MW: 449.44 **BP** (°C)**:** 636.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.122E-04	4.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.112E-04	5.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
1.112E-05	5.000E-03	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
1.335E-04	6.000E-02	25	A414	1 0 1 1 1	

4205. $C_{21}H_{24}F_3N_3S$
Trifluoperazine
Stelazine
RN: 117-89-5 **MP** (°C)**:** 232
MW: 407.50 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.223E-02	24	G022	2 0 1 1 1	
3.600E-05	1.467E-02	37	F011	1 0 1 1 1	pH 7.4

4206. $C_{21}H_{25}NO$
4-Cyano-4′-octyloxybiphenyl
8 COB
RN: **MP** (°C)**:**
MW: 307.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-07	8.301E-05	21	D300	2 2 1 1 2	

4207. $C_{21}H_{25}N_5O_5$
Benzoic acid, 4-(4-morpholinylmethyl)-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-75-5 **MP** (°C)**:**
MW: 427.46 **BP** (°C)**:** 712.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-03	7.700E-01	21	B419	1 1 2 2 1	int

4208. $C_{21}H_{26}ClN_3OS$
Perphenazine
4-(3-(2-Chlorophenothiazin-10-YL)propyl)-1-piperazineethanol
Etrafon
Trilafon
RN: 58-39-9 **MP** (°C)**:** 97
MW: 403.98 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	2.828E-02	24	G022	2 0 1 1 1	

4209. $C_{21}H_{26}FN_3O_4$
Permafloxacin
RN: 143383-65-7 **MP** (°C)**:**
MW: 403.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-02	7.477E+00	25	F415	0 0 0 0 0	Average

4210. $C_{21}H_{26}N_2O_3$
1-(2,3-Dihydro-5-methoxybenzo[b]furan-2-ylmethyl)-4-(*o*-methoxyphenyl)piperazine
RN: **MP** (°C)**:**
MW: 354.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.642E-05	2.000E-02	37	L079	1 0 1 1 0	intrinsic

4211. $C_{21}H_{26}N_2S_2$
Thioridazine
10H-Phenothiazine
10-[2-(1-Methyl-2-piperidyl)ethyl]-2-methylthio
Aldazine
Mellaril
Melleril
RN: 50-52-2 **MP** (°C)**:**
MW: 370.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	1.113E-03	22.5	B440	0 0 0 0 0	

4212. $C_{21}H_{26}O_4$
Lifibrol
Benzoic acid, 4-[4-[4-(1,1-dimethylethyl)phenyl]-2-hydroxybutoxy]-
RN: 96609-16-4 **MP** (°C)**:**
MW: 342.44 **BP** (°C)**:** 536.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.301E-04	12.0	B412	1 0 2 2 1	mod 2 crystal
8.600E-07	2.945E-04	12.0	B412	1 0 2 2 1	mod I crystal
7.000E-07	2.397E-04	20.0	B412	1 0 2 2 1	mod 2 crystal
1.110E-06	3.801E-04	20.0	B412	1 0 2 2 1	mod 1 crystal
1.070E-06	3.664E-04	29.0	B412	1 0 2 2 1	mod 2 crystal
1.640E-06	5.616E-04	29.0	B412	1 0 2 2 1	mod 1 crystal
2.090E-06	7.157E-04	38.0	B412	1 0 2 2 1	mod 2 crystal
2.740E-06	9.383E-04	38.0	B412	1 0 2 2 1	mod 1 crystal
3.080E-06	1.055E-03	47.0	B412	1 0 2 2 1	mod 2 crystal
4.890E-06	1.675E-03	47.0	B412	1 0 2 2 1	mod 1 crystal
4.690E-06	1.606E-03	54.0	B412	1 0 2 2 1	mod 2 crystal
5.900E-06	2.020E-03	54.0	B412	1 0 2 2 1	mod 1 crystal

4213. $C_{21}H_{26}O_4$
17-Hydroxy-6-methyl-16-methylenepregna-4,6-diene-3,20-dione acetate
RN: **MP** (°C)**:**
MW: 342.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-06	2.900E-03	37	H004	0 0 0 0 0	

4214. $C_{21}H_{26}O_5$
Prednisone
1,4-Pregnadiene-17α,21-diol-3,11,20-trione
1,4-Pregnadiene-17x,21-diol-3,11,20-trione
Delcortin
Metocorten
Panasol
RN: 53-03-2 **MP** (°C)**:** 234
MW: 358.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-04	1.150E-01	25	K003	2 1 1 1 1	
2.734E-04	9.799E-02	ns	B404	0 2 1 1 0	

4215. $C_{21}H_{27}FO_5$

Fluprednisolone
6α-Fluoro-11β,17,21-trihydroxypregna-1,4-diene-3,20-dione17,21-trihydroxypregna-1,4-diene-3,20-dione
Alphadrol
RN: 53-34-9 **MP** (°C)**:**
MW: 378.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-03	1.040E+00	37	H004	0 0 0 0 0	

4216. $C_{21}H_{27}FO_5.H_2O$

Fluprednisolone (monohydrate)
RN: 53-34-9 **MP** (°C)**:**
MW: 396.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	5.860E-01	37	H004	0 0 0 0 0	

4217. $C_{21}H_{27}FO_6$

Triamcinolone
9α-Fluoro-11β,16α,17α,21-tetrahydroxy-1,4-pregnadiene-3,20-dione
9α-Fluoro-16α-hydroxyprednisolone
Aristocort
RN: 124-94-7 **MP** (°C)**:** 269
MW: 394.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-04	7.999E-02	25	F024	1 0 0 0 0	
4.260E-04	1.680E-01	37	C400	2 0 2 2 2	

4218. $C_{21}H_{27}NO_3$

Propafenone
RN: 54063-53-5 **MP** (°C)**:**
MW: 341.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	7.599E-04	22.5	B440	0 0 0 0 0	

4219. $C_{21}H_{28}N_2$
1-(Diphenylmethyl)-4-butylpiperazine
RN: **MP** (°C)**:**
MW: 308.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	4.816E-01	25	M438	0 0 0 0 0	

4220. $C_{21}H_{28}N_4O_7$
Pentyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 448.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	2.646E-01	25	M316	1 1 1 1 2	

4221. $C_{21}H_{28}O_2$
Norgestrel
Microlut
Microval
RN: 797-63-7 **MP** (°C)**:** 206
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4222. $C_{21}H_{28}O_2$
Ethisterone
17α-Ethynyl testosterone
Ethynyl testosterone
Gestoral
Pregneninolone
Anhydrohydroxyprogesterone
RN: 434-03-7 **MP** (°C)**:** 269
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-06	5.999E-04	20	G072	1 2 2 1 2	
1.600E-06	4.999E-04	20	L077	1 2 2 2 1	
1.280E-06	4.000E-04	25	K003	2 1 1 1 1	
2.200E-06	6.874E-04	27.34	L077	1 2 2 2 1	
3.200E-06	9.999E-04	35	L077	1 2 2 2 1	
3.500E-06	1.094E-03	42.34	L077	1 2 2 2 1	
4.200E-06	1.312E-03	50	L077	1 2 2 2 1	

4223. $C_{21}H_{28}O_2$
1,1,1-Trimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 27955-87-9 **MP** (°C)**:**
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-07	1.400E-04	rt	C122	0 0 0 0 0	

4224. $C_{21}H_{28}O_5$
Prednisolone
11β,17α,21-Trihydroxypregna-1,4-diene-3,20-dione
Ropredlone
Predonin
Hostacortin H
Nisolone
RN: 50-24-8 **MP** (°C)**:** 240
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.173E-03	2.225E+00	25	G008	1 2 1 1 2	*sic*
5.963E-04	2.150E-01	25	K003	2 1 1 1 1	
1.379E-03	4.970E-01	25	K021	1 2 2 2 1	
5.770E-04	2.080E-01	25	M457	0 0 0 0 0	
7.000E-04	2.523E-01	30	H016	2 2 2 2 0	EFG
1.268E-03	4.570E-01	30	T002	1 0 2 0 2	anhydrous, form A
1.398E-03	5.040E-01	30	T002	1 0 2 0 2	anhydrous, form B
6.658E-04	2.400E-01	30	T002	1 0 2 0 2	hydrate
6.658E-04	2.400E-01	30	W006	2 2 2 1 2	hydrate, form C
4.694E-04	1.692E-01	37	C400	2 0 2 2 2	
9.738E-04	3.510E-01	37	H004	0 0 0 0 0	
5.500E-04	1.982E-01	ns	F327	0 0 1 2 2	
2.774E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.398E-03	5.040E-01	ns	W006	2 2 2 1 2	anhydrous, form B

4225. $C_{21}H_{28}O_5$
Aldosterone
18-Oxocorticosterone
Aldocortin
Electrocortin
18-Oxo-11β,21-dihydroxy-4-pregnene-3,20-dione
RN: 52-39-1 **MP** (°C)**:** 108
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	5.118E-02	37	H034	1 0 2 1 2	pH 7.4
1.413E-04	5.092E-02	ns	R427	0 0 0 0 0	

4226. $C_{21}H_{28}O_5$
Cortisone
17-Hydroxy-11-dehydrocorticosterone
Cortate
RN: 53-06-5 **MP** (°C)**:** 222
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.766E-04	2.799E-01	20	D041	1 0 0 0 0	
6.379E-04	2.299E-01	25	K003	2 1 1 1 1	
7.768E-04	2.800E-01	25	M023	1 0 2 1 1	
7.500E-04	2.703E-01	30	L344	2 0 1 1 0	EFG
6.000E-04	2.163E-01	37	E014	2 2 2 1 2	pH 7.3
7.768E-04	2.800E-01	ns	B338	0 0 0 0 1	

4227. $C_{21}H_{29}FO_5$
Fludrocortisone
9α-Fluoro-17-hydroxycorticosterone
9α-Fluorohydrocortisone
Florinef
RN: 127-31-1 **MP** (°C)**:** 260dec
MW: 380.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E-04	1.110E-01	25	K021	1 2 2 2 1	
8.516E-04	3.240E-01	25	L009	1 0 0 1 1	
2.411E-04	9.172E-02	37	C400	2 0 2 2 2	

4228. $C_{21}H_{29}NO$
N,*N*-Dicyclohexylcinnamamide
N,*N*-Dicyclohexyl-3-phenyl2-propenamide
RN: 6631-21-6 **MP** (°C)**:**
MW: 311.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.680E-06	1.769E-03	ns	H350	0 0 0 0 0	

4229. $C_{21}H_{29}N_3O$
Disopyramide
α-(2-(Diisopropylamino)ethyl)-α-phenyl-2-pyridineacetamide
RN: 3737-09-5 **MP** (°C)**:**
MW: 339.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.817E-05	6.170E-03	22.5	B440	0 0 0 0 0	
1.995E-02	6.774E+00	ns	R427	0 0 0 0 0	

4230. $C_{21}H_{30}N_4O_{10}$
Methylol riboflavine
Methylol-riboflavin
RN: **MP** (°C)**:**
MW: 498.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-02	1.190E+01	20	F300	1 0 0 0 2	compound not stable

4231. $C_{21}H_{30}N_6O_4S$
Benzenesulfonamide, *N*-[2-(dimethylamino)ethyl]-4-(2,3,4,5,6,7-hexahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-
RN: 89073-58-5 **MP** (°C)**:** 270dec
MW: 462.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	1.990E+01	ns	H316	0 0 0 0 0	0.1N HCL
1.081E-04	5.000E-02	ns	H316	0 0 0 0 0	pH 7.4

4232. $C_{21}H_{30}O_2$
Tetrahydrocannabinol
THC
Dronabinol
δ9-Tetrahydrocannabinol
RN: 1972-08-3 **MP** (°C)**:**
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.904E-06	2.800E-03	23	G018	1 0 0 1 0	

4233. $C_{21}H_{30}O_2$
Progesterone
δ4-Pregnene-3,20-dione
Corlutin
Corlutina
Lutein
Pregn-4-ene-3,20-dione
RN: 57-83-0 **MP** (°C)**:** 121
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-05	5.346E-03	10	B012	2 0 1 1 0	
2.200E-05	6.918E-03	20	B012	2 0 1 1 0	
3.210E-05	1.009E-02	20	L077	1 2 2 2 2	
2.600E-05	8.176E-03	21.70	M108	1 2 1 1 2	form A

(*continued*)

4233. $C_{21}H_{30}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.837E-05	1.521E-02	23	B014	0 0 1 2 2	
3.720E-05	1.170E-02	24.00	M108	1 2 1 1 2	form B
2.800E-05	8.805E-03	25	B012	2 0 1 1 0	
2.512E-05	7.899E-03	25	B041	1 0 2 2 0	EFG
3.802E-05	1.196E-02	25	F312	1 1 2 2 2	units assumed
2.862E-05	9.000E-03	25	K003	2 1 1 1 1	
6.359E-04	2.000E-01	25	P324	0 0 0 0 0	
2.810E-05	8.837E-03	25.30	M108	1 2 1 1 2	form A
3.690E-05	1.160E-02	27.34	L077	1 2 2 2 2	
3.600E-05	1.132E-02	30	B012	2 0 1 1 0	
3.498E-05	1.100E-02	30	M007	2 2 1 2 2	average of 8
3.800E-05	1.195E-02	30.20	M108	1 2 1 1 2	form A
4.520E-05	1.421E-02	30.50	M108	1 2 1 1 2	form B
4.230E-05	1.330E-02	35	L077	1 2 2 2 2	
5.390E-05	1.695E-02	35.50	M108	1 2 1 1 2	form B
4.690E-05	1.475E-02	36.40	M108	1 2 1 1 2	form A
3.816E-05	1.200E-02	37	A086	1 0 1 1 2	
3.528E-05	1.109E-02	37	C400	2 0 2 2 2	
4.800E-05	1.509E-02	37	H034	1 0 2 1 2	pH 7.4
4.260E-05	1.340E-02	37	H035	1 1 1 1 2	pH 7.4
4.007E-05	1.260E-02	37	L010	2 0 2 1 1	
4.260E-05	1.340E-02	37.50	B041	1 0 2 2 2	
3.981E-05	1.252E-02	37.50	B041	1 0 2 2 0	EFG
3.800E-05	1.195E-02	40	B012	2 0 1 1 0	
6.750E-05	2.123E-02	40.70	M108	1 2 1 1 2	form B
6.370E-05	2.003E-02	41.30	M108	1 2 1 1 2	form A
4.580E-05	1.440E-02	42.34	L077	1 2 2 2 2	
6.500E-05	2.044E-02	46.10	M108	1 2 1 1 2	form A
4.900E-05	1.541E-02	50	B012	2 0 1 1 0	
4.930E-05	1.550E-02	50	L077	1 2 2 2 2	
		amb	L434	0 0 0 0 0	
1.908E-05	6.000E-03	ns	B404	0 2 1 1 0	

4234. $C_{21}H_{30}O_3$

Deoxycorticosterone
21-Hydroxyprogesterone
4-Pregnen-21-ol-3,20-dione
11-Deoxycorticosterone
21-Hydroxypregn-4-ene-3,20-dione

RN: 64-85-7 **MP** (°C)**:** 141.5
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.387E-04	1.450E-01	25	K003	2 1 1 1 1	
4.588E-04	1.516E-01	37	C400	2 0 2 2 2	
1.800E-04	5.948E-02	37	E014	2 2 2 1 2	pH 7.3
1.070E-04	3.536E-02	37	H034	1 0 2 1 2	pH 7.4

4235. $C_{21}H_{30}O_3$
11α-Hydroxyprogesterone
11α-Hydroxy-4-pregnene-3,20-dione
RN: 80-75-1 **MP** (°C)**:**
MW: 330.47 **BP** (°C)**:** 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E-04	1.164E-01	37	C400	2 0 2 2 2	

4236. $C_{21}H_{30}O_3$
11β-Hydroxyprogesterone
11β-Hydroxypregn-4-ene-3,20-dione
RN: 600-57-7 **MP** (°C)**:**
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	3.084E-02	37	C400	2 0 2 2 2	

4237. $C_{21}H_{30}O_3$
5,6-Dehydroisoandrosterone acetate
Androst-5-en-17-one, 3-(acetyloxy)-, (3β)-
RN: 853-23-6 **MP** (°C)**:** 166
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-05	1.150E-02	ns	B057	0 2 1 1 2	

4238. $C_{21}H_{30}O_3$
Testosterone acetate
17-*O*-Acetyltestosterone
Androst-4-en-3-one, 17-(acetyloxy)-, (17β)-
RN: 1045-69-8 **MP** (°C)**:** 140
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.111E-06	2.350E-03	25	J004	1 0 1 1 2	
7.111E-06	2.350E-03	ns	B057	0 2 1 1 2	

4239. $C_{21}H_{30}O_3$
17-α-Hydroxyprogesterone
Pregn-4-ene-3,20-dione, 17-hydroxy-
Prodix
Prodox
U 3096
RN: 68-96-2 **MP** (°C)**:** 222
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-05	5.056E-03	20	L077	1 2 2 2 2	
1.960E-05	6.477E-03	27.34	L077	1 2 2 2 2	
2.760E-05	9.121E-03	35	L077	1 2 2 2 2	
3.580E-05	1.183E-02	42.34	L077	1 2 2 2 2	
4.290E-05	1.418E-02	50	L077	1 2 2 2 2	

4240. $C_{21}H_{30}O_4$
Corticosterone
11,21-Dihydroxyprogesterone
δ(4)-Pregnene-11β,21-diol-3,20-dione
11β,21-Dihydroxypregn-4-ene-3,20-dione
RN: 50-22-6 **MP** (°C)**:** 182
MW: 346.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.943E-04	2.405E-01	37	C400	2 0 2 2 2	

4241. $C_{21}H_{30}O_4$
11β,17α-Dihydroxy-4-pregnene-3,20-dione
Pregn-5-ene-3,20-dione, 11,17-dihydroxy-
Pregn-5-ene-3,20-dione, 11b,17-dihydroxy-
RN: 603-97-4 **MP** (°C)**:**
MW: 346.47 **BP** (°C)**:** 516.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.361E-04	8.180E-02	37	C400	2 0 2 2 2	

4242. $C_{21}H_{30}O_4$
Cortexolone
11-Deoxy-17-hydroxycorticosterone
11-Deoxycortisol
11-Desoxycortisone
17,21-Dihydroxy-4-pregnene-3,20-dione
17α,21-Dihydroxypregn-4-ene-3,20-dione
RN: 152-58-9 **MP** (°C)**:** 208
MW: 346.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-04	4.408E-02	37	C400	2 0 2 2 2	

4243. $C_{21}H_{30}O_5$
Hydrocortisone
11β,17,21-Trihydroxypregn-4-ene-3,20-dione
Colifoam
Cortaid
Cortef
Bactine
RN: 50-23-7 **MP** (°C)**:** 218.5
MW: 362.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.733E-01	10	B012	2 0 1 1 0	
7.725E-04	2.800E-01	20	A067	0 0 0 0 1	
7.430E-04	2.693E-01	20	B012	2 0 1 1 0	
8.109E-04	2.939E-01	22.5	B422	2 0 2 2 2	
8.820E-04	3.197E-01	25	B012	2 0 1 1 0	
9.932E-04	3.600E-01	25	C437	0 0 0 0 0	Average
7.725E-04	2.800E-01	25	H015	1 0 0 0 1	
8.194E-04	2.970E-01	25	H098	1 0 2 0 2	
8.190E-04	2.969E-01	25	H320	0 0 0 0 0	
8.194E-04	2.970E-01	25	H320	0 0 0 0 0	
7.860E-04	2.849E-01	25	K003	2 1 1 1 1	
1.614E-03	5.850E-01	25	K021	1 2 2 2 1	
7.725E-04	2.800E-01	25	M023	1 0 2 1 1	
9.896E-03	3.587E+00	25	P324	0 0 0 0 0	
1.034E-03	3.748E-01	30	B012	2 0 1 1 0	
1.000E-03	3.625E-01	30	L344	2 0 1 1 0	EFG
1.077E-03	3.905E-01	37	C400	2 0 2 2 2	
1.070E-03	3.878E-01	37	H036	1 0 2 2 2	EFG
1.265E-03	4.585E-01	40	B012	2 0 1 1 0	
1.519E-03	5.506E-01	50	B012	2 0 1 1 0	
7.725E-04	2.800E-01	298	F016	0 0 0 0 0	
1.159E-03	4.200E-01	amb	L434	0 0 0 0 0	
1.104E-03	4.000E-01	amb	L445	0 0 0 0 0	Intrinsic
7.116E-04	2.579E-01	ns	B404	0 2 1 1 0	

4244. $C_{21}H_{30}O_6$
Cortisone acetate
Pregn-4-ene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-
RN: 50-04-4 **MP** (°C)**:** 235
MW: 378.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.284E-05	2.000E-02	22.5	G301	0 0 0 0 0	
5.020E-05	1.900E-02	25	K003	2 1 1 1 1	
5.284E-05	2.000E-02	25	M023	1 0 2 1 0	
7.398E-05	2.800E-02	25	P096	0 0 0 0 0	
1.000E-04	3.785E-02	30	L068	1 0 0 1 0	EFG

4245. $C_{21}H_{31}NO$
N-Cyclododecylcinnamamide
2-Propenamide, *N*-cyclododecyl-3-phenyl
RN: 59832-03-0 **MP** (°C)**:**
MW: 313.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-08	1.226E-05	ns	H350	0 0 0 0 0	

4246. $C_{21}H_{31}N_3O_2$
2-Pentoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-pentoxyquinoline-4-carboxamide
RN: 2717-02-4 **MP** (°C)**:**
MW: 357.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-05	1.895E-02	ns	B018	0 0 0 0 1	
5.300E-05	1.895E-02	ns	M066	0 0 0 0 1	

4247. $C_{21}H_{32}O_2$
3,20-Pregnanedione
7α-17-Dimethyltestosterone
Bolasterone
RN: 128-23-4 **MP** (°C)**:**
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-04	5.800E-02	37	H004	0 0 0 0 0	

4248. $C_{21}H_{32}O_2$
7α,17-Dimethyl-19-nortestosterone
RN: **MP** (°C)**:**
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-04	4.540E-02	37	H004	0 0 0 0 0	

4249. $C_{21}H_{32}O_2$
Pregnenolone
3β-Hydroxy-5-pregnen-20-one
5-Pregnen-3β-ol-20-one
3β-Hydroxypregn-5-en-20-one
RN: 145-13-1 **MP** (°C)**:** 193
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E-05	7.058E-03	37	H034	1 0 2 1 2	pH 7.4
9.479E-05	3.000E-02	amb	L434	0 0 0 0 0	
1.295E-04	4.100E-02	rt	B408	0 0 2 2 2	

4250. $C_{21}H_{32}O_3$
Androstanolone acetate
Androstan-3-one, 17-(acetyloxy)-, (5α,17β)-
Stanolone acetate
RN: 1164-91-6 **MP** (°C)**:**
MW: 332.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-01	8.884E+01	ns	B057	0 2 1 1 2	

4251. $C_{21}H_{33}NO$
2-Propenamide, *N*-dodecyl-3-phenyl-
RN: 55125-24-1 **MP** (°C)**:**
MW: 315.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-06	6.626E-04	ns	H350	0 0 0 0 0	

4252. $C_{21}H_{33}NO_7$
Lasiocarpine
(7α-Angelyloxy-5,6,7,8α-tetrahydro-3H-pyrrolizin-1-yl)methyl-2,3-dihydroxy-2-(1′-methoxyethyl)-3-methylbutyrate
RN: 303-34-4 **MP** (°C)**:** 97
MW: 411.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-02	6.754E+00	ns	I312	0 0 0 0 0	

4253. $C_{21}H_{34}O_2$
Pregnanolone
3-Deoxo-3a-hydroxy-5b-dihydroprogesterone
3a,5b-Tetrahydroprogesterone
3a-Hydroxy-5b-pregnan-20-one
Pregnan-3a-ol-20-one
3a,5b-Pregnanolone
RN: 128-20-1 **MP** (°C)**:**
MW: 318.50 **BP** (°C)**:** 431.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-05	8.000E-03	rt	B408	0 0 2 2 2	

4254. $C_{21}H_{34}O_3$
Tetradecyl *p*-hydroxybenzoate
Tetradecyl 4-hydroxybenzoate
RN: 71177-53-2 **MP** (°C)**:**
MW: 334.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-03	3.639E-01	25	D081	1 2 2 1 2	

4255. $C_{21}H_{35}NO_3$
4-Octoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-76-1 **MP** (°C)**:**
MW: 349.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.398E-02	ns	M066	0 0 0 0 1	

4256. $C_{21}H_{36}O_4$
4-Nonylphenol triethoxylate
Ethanol, 2-[2-[2-(4-nonylphenoxy)ethoxy]ethoxy]-
RN: 51437-95-7 **MP** (°C)**:**
MW: 352.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-05	5.880E-03	20.5	A335	0 0 0 0 0	
1.670E-05	5.887E-03	20.5	A335	0 0 0 0 0	

4257. $C_{21}H_{40}O_4$
α-Monoolein
1-Monoolein
Glycerol monooleate
9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol
1-Oleoyl-*sn*-glycerol
RN: 25496-72-4 **MP** (°C)**:**
MW: 356.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<3.57E-03	30	O321	0 0 0 0 0	

4258. $C_{21}H_{44}$
3-Methyleicosane
18-Methyleicosane
RN: 6418-46-8 **MP** (°C)**:**
MW: 296.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.294E-13	1.570E-10	23	C332	0 0 0 0 0	

4259. $C_{21}H_{44}$
2-Methyleicosane
19-Methyleicosane
RN: 1560-84-5 **MP** (°C)**:**
MW: 296.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.091E-13	1.510E-10	23	C332	0 0 0 0 0	

4260. $C_{22}H_{12}$
Indeno(1,2,3-cd)pyrene
Indeno[1,2,3-cd]pyrene
o-Phenylenepyrene
RN: 193-39-5 **MP** (°C)**:** 162.5
MW: 276.34 **BP** (°C)**:** 536

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.876E-10	1.900E-07	ns	W302	0 0 0 0 1	

4261. $C_{22}H_{12}$
Benzo[g,h,i]perylene
Benz[g,h,i]perylene
RN: 191-24-2 **MP** (°C)**:** 279
MW: 276.34 **BP** (°C)**:** >500

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.958E-10	1.370E-07	25	D406	1 2 2 2 2	
6.500E-10	1.796E-07	25	K123	1 0 2 2 1	
9.409E-10	2.600E-07	25	M064	1 1 2 2 1	
9.400E-10	2.598E-07	25	M342	1 0 1 1 1	
9.409E-10	2.600E-07	ns	M344	0 0 0 0 1	
2.533E-09	7.000E-07	ns	W302	0 0 0 0 0	

4262. $C_{22}H_{14}$
Picene
1,2,7,8-Dibenzphenanthrene
3,4-Benzchrysene
RN: 213-46-7 **MP** (°C)**:** 366
MW: 278.36 **BP** (°C)**:** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-08	4.315E-06	20	E009	1 0 0 1 2	
8.981E-09	2.500E-06	27	D003	1 0 0 1 1	

4263. $C_{22}H_{14}$
1,2:3,4-Dibenzanthracene
RN: 215-58-7 **MP** (°C)**:** 205
MW: 278.36 **BP** (°C)**:** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-09	1.600E-06	25	B319	2 0 1 2 1	
8.200E-08	2.283E-05	25	K123	1 0 2 2 1	

4264. $C_{22}H_{14}$
1,2:7,8-Dibenzanthracene
Dibenz[a,j]anthracene
Dinaphthanthracene
RN: 224-41-9 **MP** (°C)**:** 196
MW: 278.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-08	8.629E-06	25	K123	1 0 2 2 1	
4.311E-08	1.200E-05	27	D003	1 0 0 1 1	

4265. $C_{22}H_{14}$
1,2:5,6-Dibenzanthracene
1,2,5,6-Dibenzanthracene
RN: 53-70-3 **MP** (°C)**:** 266
MW: 278.36 **BP** (°C)**:** 524

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.945E-09	2.490E-06	24	H106	1 0 2 2 2	
7.904E-09	2.200E-06	25	B319	2 0 1 2 2	
2.150E-09	5.985E-07	25	K001	2 2 2 2 2	
1.100E-07	3.062E-05	25	K123	1 0 2 2 1	*sic*
8.945E-09	2.490E-06	25	M156	1 2 1 1 2	
1.800E-09	5.010E-07	25	M342	1 0 1 1 2	
1.796E-09	5.000E-07	27	D003	1 0 0 1 1	

4266. $C_{22}H_{16}F_3N_3$
Fluotrimazole
1H-1,2,3-Triazole, 1-[diphenyl[3-(trifluoromethyl)phenyl]methyl]-
RN: 57381-79-0 **MP** (°C)**:** 132
MW: 379.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E-09	1.500E-06	20	M161	1 0 0 0 1	

4267. $C_{22}H_{16}O_8$
Ethyl biscoumacetate
Tromexan
RN: 548-00-5 **MP** (°C)**:** 154
MW: 408.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.179E-04	8.900E-02	20	K028	2 1 2 1 2	pH 3.8, form I
3.747E-04	1.530E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.179E-04	8.899E-02	20	M042	1 0 0 0 1	pH 3.8, form I, mp 172-182 C
3.761E-04	1.536E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 153-160 C

4268. $C_{22}H_{17}ClN_2$
Clotrimazole
1-(*o*-Chloro-α,α-diphenylbenzyl)imidazole
1-[α-(2-Chlorophenyl)benzhydryl]imidazole
Lotrimin
RN: 23593-75-1 **MP** (°C)**:** 147–149
MW: 344.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.90E-05	<1.00E-02	25	H328	0 0 0 0 0	
8.700E-05	3.000E-02	amb	L434	0 0 0 0 0	

4269. $C_{22}H_{18}N_2O_4S$
Hydantoin, 5,5-diphenyl-1-(*o*-tolylsulfonyl)-
1-(*o*-Methylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-41-9 **MP** (°C)**:**
MW: 406.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-06	7.600E-04	37	F183	1 0 1 1 2	intrinsic

4270. $C_{22}H_{18}N_2O_5S$
1-(*p*-Methoxylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-37-3 **MP** (°C)**:**
MW: 422.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-06	5.100E-04	37	F183	1 0 1 1 2	intrinsic

4271. $C_{22}H_{19}Br_2NO_3$
Deltamethrin
3-(2,2-Dibromoethenyl)-2,2-dimethylcyclopropanecarboxylic acid, cyano(3-phenoxyphenyl) methyl ester
RN: 52918-63-5 **MP** (°C)**:** 98–101
MW: 505.22 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-09	2.000E-06	25	M364	1 0 0 0 1	
3.959E-09	2.000E-06	ns	V414	0 0 0 0 0	

4272. $C_{22}H_{19}F_6NOS$
α-Piperidyl-3,6-bis(trifluoromethyl)-9-phenanthrenemethanol
RN: 31817-24-0 **MP** (°C)**:** 215
MW: 459.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E-05	7.500E-03	25	A013	1 0 2 2 0	average

4273. $C_{22}H_{20}$
10-Butyl-1,2-benzanthracene
RN: 188124-94-9 **MP** (°C)**:** 97
MW: 284.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-08	8.000E-06	27	D003	1 0 0 1 1	

4274. $C_{22}H_{20}Cl_2N_2O_3$
Benzofenap
2-((4-(2,4-Dichloro-3-methylbenzoyl)-1,3-dimethyl-1H-pyrazol-5-yl)oxy)-1-(4-methylphenyl) ethanone
RN: 82692-44-2 **MP** (°C)**:**
MW: 431.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-07	1.303E-04	ns	R427	0 0 0 0 0	

4275. $C_{22}H_{20}O_{13}$
Carminic acid
Carmine
Carminsaeure
RN: 1260-17-9 **MP** (°C)**:**
MW: 492.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.637E-03	1.298E+00	rt	D021	0 0 1 1 1	

4276. $C_{22}H_{22}ClN_3O_5$

Propaquizafop
2-[(Isopropylideneamino)oxy]ethyl (*R*)-2-[*p*-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-propionate
(*R*)-2-{[(1 Methylethylidene)amino]oxy}ethyl 2-{4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy} propanoate
Agil
Shogun
RO 17-3664
RN: 111479-05-1 **MP** (°C)**:**
MW: 443.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-06	6.270E-04	ns	R427	0 0 0 0 0	

4277. $C_{22}H_{22}FN_3O_2$

Droperidol
2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro-
Sintodril
Neurolidol
R 4749
RN: 548-73-2 **MP** (°C)**:**
MW: 379.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-05	4.100E-03	30	P044	0 0 0 0 0	

4278. $C_{22}H_{22}N_2O_4$

N,*N*′-Dibutyl-1,4,5,8-naphthalenediimide
Benzo[*lmn*][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-dibutyl-
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide, *N*,*N*′-dibutyl-
RN: 17655-95-7 **MP** (°C)**:**
MW: 378.43 **BP** (°C)**:** 572.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.892E-06	23	B410	2 1 2 2 2	

4279. $C_{22}H_{22}N_2O_8$
Methacycline base
Oxytetracycline, 6-methylene-
Tri-methacycline
Rondomycin
RN: 914-00-1 **MP** (°C)**:**
MW: 442.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.706E-02	7.548E+00	21	M044	2 0 2 2 2	

4280. $C_{22}H_{22}N_4O_6$
Benzoyl-mitomycin C
RN: **MP** (°C)**:**
MW: 438.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	4.384E-03	25	M316	1 1 1 1 2	

4281. $C_{22}H_{23}ClN_2O_8$
Chlortetracycline
7-Chlortetracycline
Acronize PD
Acronize
RN: 57-62-5 **MP** (°C)**:**
MW: 478.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-03	6.300E-01	25	B191	1 0 0 0 1	
2.297E-03	1.100E+00	37	M104	1 2 1 1 0	form II, EFG, recrystallized
1.566E-03	7.500E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized
2.088E-04	1.000E-01	37	M105	1 2 1 1 0	EFG

4282. $C_{22}H_{23}NO_3$
Fenpropanate
Danitol
Herald
WL 41706
Miothrin
2,2,3,3-Tetramethylcyclopropane carboxylic acid, cyano(3-phenoxyphenyl)methyl ester
RN: 39515-41-8 **MP** (°C)**:**
MW: 349.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-08	1.424E-05	ns	R427	0 0 0 0 0	

4283. $C_{22}H_{23}NO_7$
Noscapine
Narcotine
O-Methylnarcotoline
Opianin
Opian
RN: 128-62-1 **MP** (°C)**:** 176
MW: 413.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.654E-02	15	K059	2 2 2 0 0	
7.327E-04	3.029E-01	25	D004	0 0 0 0 0	
7.256E-04	3.000E-01	30	A073	1 1 1 1 0	
1.693E-03	7.000E-01	40	A073	1 1 1 1 0	
2.419E-03	1.000E+00	50	A073	1 1 1 1 1	
2.419E-03	1.000E+00	60	A073	1 1 1 1 1	
2.419E-03	1.000E+00	70	A073	1 1 1 1 1	
2.419E-03	1.000E+00	80	A073	1 1 1 1 1	
3.628E-03	1.500E+00	90	A073	1 1 1 1 1	
4.838E-03	2.000E+00	100	A073	1 1 1 1 1	

4284. $C_{22}H_{24}ClN_5O_2$
Domperidone
5-Chloro-1-[1-[3-(2-oxo-1-benzimidazolinyl)propyl]-4-piperidyl]-2-benzimidazolinone
RN: 57808-66-9 **MP** (°C)**:** 242.5
MW: 425.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-05	1.710E-02	22	J420	0 0 0 0 0	pH6.5

4285. $C_{22}H_{24}N_2O_8$

Tetracycline
Achromycin V
Sumycin
Robitet
Panmycin

RN: 60-54-8 **MP** (°C)**:** 176dec
MW: 444.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.900E-04	4.400E-01	25	B191	1 0 0 0 1	neutral pH
5.200E-04	2.311E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
5.700E-04	2.533E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
2.655E-03	1.180E+00	29	N031	1 2 2 2 0	EFG, pH 5.0
7.600E-04	3.378E-01	30	L069	1 0 1 1 0	EFG
1.777E-03	7.900E-01	35	N031	1 2 2 2 0	EFG, pH 5.0
7.875E-02	3.500E+01	37	M104	1 2 1 1 2	form II, recrystallized
6.232E-02	2.770E+01	37	M104	1 2 1 1 2	form I, recrystallized
6.478E-04	2.879E-01	ns	N302	0 2 1 2 2	

4286. $C_{22}H_{24}N_2O_8.H_2O$

Doxycycline (monohydrate)
Doxylin
Monodox
Vibra-tabs
Doxy-caps
Vibramycin

RN: 564-25-0 **MP** (°C)**:** 201dec
MW: 462.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.362E-03	6.300E-01	25	B132	2 1 1 1 0	EFG

4287. $C_{22}H_{24}N_2O_9$

Oxytetracycline
Glomycin
Hydroxytetracycline
Riomitsin
Terrafungine
Stevacin

RN: 79-57-2 **MP** (°C)**:** 184
MW: 460.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.234E-04	1.950E-01	20	L051	1 0 0 0 2	
9.990E-04	4.600E-01	25	B191	1 0 0 0 1	neutral pH

(*continued*)

4287. $C_{22}H_{24}N_2O_9$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	2.210E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
6.798E-04	3.130E-01	25	H005	1 0 1 2 2	Ph 5.8
5.000E-04	2.302E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
6.515E-04	3.000E-01	29	N031	1 2 2 2 0	EFG, pH 5.0
8.687E-04	4.000E-01	37	M104	1 2 1 1 0	form II, EFG, recrystallized
6.515E-04	3.000E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized

4288. $C_{22}H_{24}N_4O_5$

Benzyl-mitomycin C

RN: **MP** (°C)**:**

MW: 424.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	6.324E-01	25	M316	1 1 1 1 2	

4289. $C_{22}H_{24}N_4O_5S$

Methanesulfonamide, *N*-[1′-[2-(2,1,3-benzoxadiazol-5-yl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4′-piperidin]-6-yl]-

Methanesulfonamide, *N*-[1′-[2-(5-benzofurazanyl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4′-piperidin]-6-yl]-

RN: **MP** (°C)**:**

MW: 456.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.752E-05	8.000E-03	22	D405	1 1 2 2 2	Intrinsic

4290. $C_{22}H_{25}NO_6$

Colchicine

Colchicin

RN: 64-86-8 **MP** (°C)**:**

MW: 399.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-02	3.846E+01	20	D041	1 0 0 0 0	
1.088E-01	4.348E+01	25	D004	0 0 0 0 0	
8.261E-02	3.300E+01	ns	K444	0 0 0 0 0	

4291. $C_{22}H_{26}F_3N_3OS$
Fluphenazine
Permitil
Modecate
Prolixin
RN: 69-23-8 **MP** (°C)**:** <25
MW: 437.53 **BP** (°C)**:** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-05	3.106E-02	37	F011	1 0 1 1 1	pH 7.4

4292. $C_{22}H_{26}N_2O_9$
Doxycycline
4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamide monohydrate
Doryx
Doxylin
Monodox
Vibramycin
RN: 564-25-0 **MP** (°C)**:**
MW: 462.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E+00	1.087E+03	25	B443	0 0 0 0 0	
2.162E-04	1.000E-01	ns	K444	0 0 0 0 0	

4293. $C_{22}H_{27}ClN_2O_4S$
Diltiazem hydrochloride
1,5-Benzothiazepin-4(5H)one,3-(acetyloxy)-5-(2-(dimethylamino)ethyl)-2,3-dihydro-2-(4-methoxyphenyl)-,
Dilacor XR
Cardizem
Cardcal
Coras
RN: 33286-22-5 **MP** (°C)**:**
MW: 450.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.131E-03	5.100E-01	25	A412	1 0 2 2 1	int

4294. $C_{22}H_{27}NO_2$
Danazol
17α-Pregna-2,4-dien-20-yno[2,3-d]isoxazol-17-ol
Danocrine
Cyclomen
RN: 17230-88-5 **MP** (°C)**:**
MW: 337.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-06	5.800E-04	25	E409	0 0 0 0 0	
1.245E-06	4.200E-04	37	S446	0 0 0 0 0	

4295. $C_{22}H_{28}F_2O_5$
Flumethasone
Flumethasonpivalate
RN: 2135-17-3 **MP** (°C)**:**
MW: 410.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.436E-06	1.000E-03	20	A067	0 0 0 0 0	

4296. $C_{22}H_{28}N_2O$
Fentanyl
1-Phenethyl-4-(phenylpropionylamino)piperidine
N-(1-Phenethyl-4-piperidyl)propionanilide
Duragesic
RN: 437-38-7 **MP** (°C)**:**
MW: 336.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.944E-04	2.000E-01	25	R338	0 0 0 0 0	
3.566E-05	1.200E-02	35	R418	0 0 0 0 0	Intrinsic

4297. $C_{22}H_{28}N_6O_3S$
Delavirdine
1-[3-[(1-Methylethyl)amino]-2-pyridinyl]-4-[[5-[(methylsulfonyl)amino]-1H-indol-2-yl]carbonyl] piperazine
1-(5-Methanesulfonamido-1H-indol-2-ylcarbonyl)-4-[3-(1-methylethylamino)pyridinyl]piperazine
1-[3-(Isopropylamino)-2-pyridyl]-4-[(5-methanesulfonamidoindol-2-yl)carbonyl]piperazine
RN: 136817-59-9 **MP** (°C)**:**
MW: 456.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.571E-02	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic

4298. $C_{22}H_{28}O_3$
Canrenone
17-Hydroxy-3-oxo-17α-pregna-4,6-diene-21-carboxylic acid lactone
RN: 976-71-6 **MP** (°C)**:** 149-151
MW: 340.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-07	2.724E-04	25	G017	1 0 1 0 0	EFG
8.100E-05	2.758E-02	37	C004	0 0 0 0 0	*sic*
8.958E-07	3.050E-04	37	O306	1 0 2 2 2	
6.374E-07	2.170E-04	rt	O306	0 0 2 2 2	

4299. $C_{22}H_{28}O_3$
Norethindrone acetate
Norethisterone acetate
RN: 51-98-9 **MP** (°C)**:** 161
MW: 340.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.288E-06	3.162E-03	10	L078	1 0 1 2 0	EFG
1.312E-05	4.467E-03	20	L078	1 0 1 2 0	EFG
1.570E-05	5.345E-03	25	H099	1 0 2 2 2	
1.652E-05	5.623E-03	25	L078	1 0 1 2 2	
1.853E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
2.937E-05	1.000E-02	40	L078	1 0 1 2 0	EFG

4300. $C_{22}H_{29}FO_4$
Fluorometholone
9-Fluoro-11β,17-dihydroxy-6α-methylpregna-1,4-diene-3,20-dione
21-Desoxy-9α-fluoro-6α-methyl-prednisolone
RN: 426-13-1 **MP** (°C)**:**
MW: 376.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.968E-05	3.000E-02	25	G008	1 2 1 1 0	

4301. $C_{22}H_{29}FO_5$
Betamethasone
Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11β,16β)-
RN: 378-44-9 **MP** (°C)**:** 230
MW: 392.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-04	5.800E-02	25	K003	2 1 1 1 1	
1.936E-04	7.599E-02	25	P096	0 0 0 0 0	

(*continued*)

4301. $C_{22}H_{29}FO_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	5.887E-02	30	O321	0 0 0 0 0	
1.529E-04	6.000E-02	30	O321	0 0 0 0 0	
1.605E-04	6.301E-02	37	C400	2 0 2 2 2	
1.605E-04	6.300E-02	ns	B404	0 2 1 1 0	
1.575E-04	6.180E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

4302. $C_{22}H_{29}FO_5$

Dexamethasone

Dexamethasone alcohol

RN: 50-02-2 **MP** (°C)**:** 262

MW: 392.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	3.218E-02	10	B012	2 0 1 1 0	
1.580E-04	6.201E-02	20	B012	2 0 1 1 0	
2.800E-04	1.099E-01	23	L345	1 0 1 1 2	
2.270E-04	8.909E-02	25	B012	2 0 1 1 0	
2.140E-04	8.399E-02	25	K003	2 1 1 1 1	
3.083E-04	1.210E-01	25	K021	1 2 2 2 1	
2.548E-04	1.000E-01	25	P312	0 0 0 0 0	
2.520E-04	9.890E-02	30	B012	2 0 1 1 0	
2.344E-04	9.200E-02	37	C400	2 0 2 2 2	
2.955E-04	1.160E-01	37	D026	0 0 0 0 0	
3.560E-04	1.397E-01	40	B012	2 0 1 1 0	
4.600E-04	1.805E-01	50	B012	2 0 1 1 0	
4.077E-04	1.600E-01	amb	L434	0 0 0 0 0	
2.548E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.707E-04	6.700E-02	ns	N302	0 2 1 2 1	

4303. $C_{22}H_{29}NO_7S_2$

Methyl *O*-acetyl-3-(acetyloxy)-*N*-{5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: **MP** (°C)**:**

MW: 483.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.817E-04	2.329E-01	ns	S453	0 0 0 0 0	

4304. $C_{22}H_{30}ClNO_2$

Propoxyphene hydrochloride
D-Propoxyphene hydrochloride
RN: 1639-60-7 **MP** (°C)**:**
MW: 375.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.842E-06	3.700E-03	25	A412	1 0 2 2 1	int

4305. $C_{22}H_{30}Cl_2N_{10}$

Chlorhexidin
Chlorhexidine
bis(5-(*p*-Chlorophenyl)biguanidinio)hexane
RN: 55-56-1 **MP** (°C)**:**
MW: 505.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.583E-04	7.999E-02	20	D341	0 0 0 0 0	
8.309E-05	4.200E-02	22.5	G301	0 0 0 0 0	

4306. $C_{22}H_{30}N_2O_2$

Aspidospermine
Aspidospermidine, 1-acetyl-17-methoxy-
RN: 466-49-9 **MP** (°C)**:** 208
MW: 354.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.701E-04	1.666E-01	c	D004	0 0 0 0 0	

4307. $C_{22}H_{30}N_2O_2S$

Sufentanil
N-[4-(Methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidyl]propionanilide
Sufenta
RN: 56030-54-7 **MP** (°C)**:**
MW: 386.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-04	7.600E-02	25	R338	0 0 0 0 0	
3.363E-06	1.300E-03	35	R418	0 0 0 0 0	Intrinsic

4308. $C_{22}H_{30}O_5$
Methylprednisolone
6α-Methylprednisolone
Medrol
Solumedrol
Metrisone
Promacortine
RN: 83-43-2 **MP** (°C)**:** 232.5
MW: 374.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.204E-04	1.200E-01	25	A014	1 0 1 1 0	EFG
2.403E-04	9.000E-02	25	A014	1 0 1 1 0	EFG, pH 5.0
2.534E-03	9.491E-01	25	G008	1 2 1 1 1	
3.445E-04	1.290E-01	25	K021	1 2 2 2 1	
1.335E-04	5.000E-02	27.14	H026	1 0 2 1 0	EFG, form I
1.923E-04	7.199E-02	30.0	H010	2 2 1 1 1	
4.273E-04	1.600E-01	31.72	H026	1 0 2 1 0	EFG, form II
3.124E-04	1.170E-01	37	H004	0 0 0 0 0	polymorph I
3.765E-04	1.410E-01	37	H004	0 0 0 0 0	polymorph II
5.341E-04	2.000E-01	40.32	H026	1 0 2 1 0	EFG, form II
2.937E-04	1.100E-01	40.32	H026	1 0 2 1 0	EFG, form I
4.273E-04	1.600E-01	51.52	H026	1 0 2 1 0	EFG, form I
1.362E-03	5.100E-01	81.45	H026	1 0 2 1 0	EFG, form II
1.068E-03	4.000E-01	81.45	H026	1 0 2 1 0	EFG, form I
2.670E-04	1.000E-01	ns	M169	0 0 0 0 1	

4309. $C_{22}H_{30}O_6$
5,16-β-Dihydroxy-6-β-methyl-3,11-dioxo-5-α-pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester
U-20235
RN: **MP** (°C)**:**
MW: 390.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.402E-04	2.500E-01	ns	K029	0 0 2 1 1	

4310. $C_{22}H_{32}O_3$
Nandrolone butyrate
RN: **MP** (°C)**:**
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-05	5.030E-03	37	C026	0 0 0 0 0	

4311. $C_{22}H_{32}O_3$
Methyltestosterone acetate
17-α-Methyltestosterone acetate
RN: 1099-79-2 **MP** (°C)**:** 164
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-05	4.926E-03	25	H099	1 0 2 2 2	
5.196E-06	1.790E-03	ns	B057	0 2 1 1 2	

4312. $C_{22}H_{32}O_3$
5,6-Dehydroisoandrosterone propionate
RN: 1167-87-9 **MP** (°C)**:**
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-05	8.320E-03	ns	B057	0 2 1 1 2	

4313. $C_{22}H_{32}O_3$
Testosterone propionate
17-(1-Oxopropoxy)-(17β)-androst-4-en-3-one
Testosterone-17-propionate
Agovirin
Androsan
Androgen
RN: 57-85-2 **MP** (°C)**:** 120
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.891E-02	20	F012	1 0 1 1 1	
4.300E-06	1.481E-03	25	J004	1 0 1 1 2	
5.806E-06	2.000E-03	25	K003	2 1 1 1 1	
6.096E-06	2.100E-03	30	T005	2 0 2 2 1	
1.060E-05	3.652E-03	37.50	B054	1 0 1 1 2	
4.296E-06	1.480E-03	ns	B057	0 2 1 1 2	

4314. $C_{22}H_{33}N_3O_2$
2-Hexoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-hexoxyquinoline-4-carboxamide
RN: 2717-03-5 **MP** (°C)**:**
MW: 371.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-06	2.489E-03	ns	B018	0 0 0 0 1	
6.700E-06	2.489E-03	ns	M066	0 0 0 0 1	

4315. $C_{22}H_{34}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-tetradecyl ester
RN: 65267-96-1 **MP** (°C)**:**
MW: 417.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-05	4.848E-03	ns	M120	0 0 1 1 2	

4316. $C_{22}H_{34}N_6O_4$
2,5-Diaziridinyl-3,6-di(1′-piperazineethanol)-1,4-benzoquinone
RN: 59886-40-7 **MP** (°C)**:** 170
MW: 446.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-02	2.000E+01	rt	C317	0 0 0 0 0	

4317. $C_{22}H_{34}O_3$
Androstanolone propionate
Androstan-3-one, 17-(1-oxopropoxy)-, (5α,17β)-
RN: 855-22-1 **MP** (°C)**:**
MW: 346.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E-06	6.200E-04	ns	B057	0 2 1 1 2	

4318. $C_{22}H_{35}NO_3$
Acetaminophen myristate
Acetaminophen tetradecanoate
RN: 54942-39-1 **MP** (°C)**:** 114
MW: 361.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-05	6.000E-03	25	B010	1 1 1 1 0	

4319. $C_{22}H_{37}NO_2$
Anandamide
Arachidonoylethanolamide
AEA
RN: 94421-68-8 **MP** (°C)**:**
MW: 347.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.188E-06	4.130E-04	25	J414	0 0 0 0 0	Intrinsic

4320. $C_{22}H_{38}O_5$
4-Octylphenol tetraethoxylate
Ethanol, 2-[2-[2-[2-(4-octylphenoxy)ethoxy]ethoxy]ethoxy]-
RN: 51437-92-4 **MP** (°C)**:**
MW: 382.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.404E-05	2.450E-02	20.5	A335	0 0 0 0 0	
6.410E-05	2.452E-02	20.5	A335	0 0 0 0 0	

4321. $C_{22}H_{39}O_3P$
Diisooctyl phenyl phosphonate
RN: **MP** (°C)**:**
MW: 382.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.61E-04	<1.00E-01	25	B070	1 2 0 1 0	

4322. $C_{22}H_{39}O_3P$
Dioctyl phenyl phosphonate
Di-*n*-octyl phenylphosphonate
DOPP
RN: 1754-47-8 **MP** (°C)**:**
MW: 382.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.23E-04	<2.00E-01	25	B070	1 2 0 1 0	

4323. $C_{22}H_{42}O_4$
Dioctyl adipate
bis(2-Ethylhexyl) adipate
RN: 103-23-1 **MP** (°C)**:**
MW: 370.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.095E-06	3.000E-03	25	F067	1 0 2 2 1	

4324. $C_{22}H_{43}N_5O_{13}$
Amikacin
Antibiotic BB-K8
RN: 37517-28-5 **MP** (°C)**:** 203
MW: 585.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-01	1.850E+02	25	K044	1 0 0 0 2	pH 10.4

4325. $C_{23}H_{16}O_6$
Pamoic acid
4,4′-Methylenebis[3-hydroxy-2-naphthalenecarboxylic acid]
3,3′-Dihydroxy-4,4′-methylenedi-2-naphthoic acid
Embonic acid
RN: 130-85-8 **MP** (°C)**:**
MW: 388.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	1.087E+02	ns	F007	0 0 0 0 1	

4326. $C_{23}H_{18}F_2N_4O$
α-(2,4-Difluorophenyl)-α-(1-2-(2-pyridyl)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
XD405
RN: 124669-93-8 **MP** (°C)**:**
MW: 404.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.418E-06	3.000E-03	22	M372	1 2 1 1 1	intrinsic

4327. $C_{23}H_{20}N_2O_2S$
G-1
p-Phenylthioethylphenylbutazone
1,2-Diphenyl-4-(2-phenylthioethyl)-3,5-pyrazolidinedione
RN: 3736-92-3 **MP** (°C)**:**
MW: 388.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.118E-03	1.600E+00	ns	B158	0 0 0 0 1	pH 7.0

4328. $C_{23}H_{20}N_2O_3S$
Sulfinpyrazone
Sulfoxyphenyl pyrazolidine
Sulfinpyrazole
1,2-Diphenyl-4-(2-(phenylsulfinyl)ethyl)-3,5-pyrazolidinedione
Anturane
RN: 57-96-5 **MP** (°C)**:**
MW: 404.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.431E-03	2.601E+00	22	J420	0 0 0 0 0	pH6.5

4329. $C_{23}H_{22}$
10-Amyl-1,2-benzanthracene
RN: 188124-96-1 **MP** (°C)**:**
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.681E-09	8.000E-07	27	D003	1 0 0 1 0	

4330. $C_{23}H_{22}O_6$
Rotenone
Tubatoxin
Derris
1,2,12,12α-Tetrahydro-2α-isopropenyl-8,9-dimethoxy(1)benzopyrano(3,4-b)furo(2,3-h)(1) benzopyran-6(6α H)-one
RN: 83-79-4 **MP** (°C)**:** 163
MW: 394.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-07	1.700E-04	25	C100	1 0 2 1 1	
3.803E-05	1.500E-02	100	M161	1 0 0 0 1	

4331. $C_{23}H_{23}NO$
Trifenmorph
Frescon
N-Tritylmorpholine
RN: 1420-06-0 **MP** (°C)**:** 175
MW: 329.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E-08	2.000E-05	20	M161	1 0 0 0 1	

4332. $C_{23}H_{24}N_4O_2$
Diantipyrylmethane
4,4′-Methylenediantipyrine
4,4′-Diantipyrylmethane
RN: 1251-85-0 **MP** (°C)**:** 182
MW: 388.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-03	4.390E-01	20	P054	0 0 0 0 0	
1.132E-03	4.398E-01	20	P054	0 0 0 0 0	

4333. $C_{23}H_{24}N_4O_6$
Benzylcarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 452.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	1.014E+00	25	M316	1 1 1 1 2	

4334. $C_{23}H_{24}N_4O_7$
Benzyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 468.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-04	2.436E-01	25	M316	1 1 1 1 2	

4335. $C_{23}H_{24}N_4S_2$
Dithiodiantipyrinylmethane
3H-Pyrazole-3-thione, 4,4′-methylenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 53799-78-3 **MP** (°C)**:** 166
MW: 420.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.103E-01	ns	D087	0 2 0 0 1	

4336. $C_{23}H_{25}N$
Fendiline
RN: 13042-18-7 **MP** (°C)**:**
MW: 315.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.389E-06	2.331E-03	22.5	B440	0 0 0 0 0	

4337. $C_{23}H_{26}FN_3O_2$
Spiperone
8-[4-(4-Fluorophenyl)-4-oxobutyl]-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one
RN: 749-02-0 **MP** (°C)**:** 192 C
MW: 395.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.091E-05	3.200E-02	22	J420	0 0 0 0 0	pH6.5

4338. $C_{23}H_{26}N_2O_4$
Brucine
Brucin
RN: 357-57-3 **MP** (°C)**:** 178
MW: 394.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.112E-03	3.200E+00	15	F300	1 0 0 0 1	
1.330E-03	5.247E-01	15	K059	2 2 2 0 2	
1.698E-02	6.700E+00	100	F300	1 0 0 0 1	
1.267E-03	4.998E-01	rt	D021	0 0 1 1 1	

4339. $C_{23}H_{26}N_2O_4.4H_2O$
Brucine (tetrahydrate)
Strychnidin-10-one, 2,3-dimethoxy-, tetrahydrate
RN: 5892-11-5 **MP** (°C)**:** 105
MW: 466.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.677E-03	3.115E+00	c	D004	0 0 0 0 0	
1.420E-02	6.623E+00	h	D004	0 0 0 0 0	

4340. $C_{23}H_{26}O_3$
Phenothrin
(3-Phenoxylphenyl)methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate
Sumithrin
3-Phenoxybenzyl D-*cis* and *trans*-2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate
RN: 26002-80-2 **MP** (°C)**:** <25
MW: 350.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	2.000E-03	30	M161	1 0 0 0 0	

4341. $C_{23}H_{27}ClO_4$
Delmadinone acetate
Pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6-chloro-
RN: 13698-49-2 **MP** (°C)**:** 168
MW: 402.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-05	6.070E-03	37	K070	1 0 0 1 2	
1.134E-05	4.570E-03	ns	K070	1 0 0 1 2	

4342. $C_{23}H_{27}FN_4O_2$
Risperidal
3-(2-(4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl)ethyl)-6,7,8,9-tetrahydro-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one
Risperidone
RN: 106266-06-2 **MP** (°C)**:**
MW: 410.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	4.474E-02	25	E406	0 0 0 0 0	
<2.44E-04	<1.00E-01	rt	B435	0 0 0 0 0	

4343. $C_{23}H_{27}NO_8$
Narceine
o-Veratric acid, 6-[[6-[2-(dimethylamino)ethyl]-2-methoxy-3,4-(methylenedioxy)phenyl]acetyl]-
NIH 10760
RN: 131-28-2 **MP** (°C)**:** 138
MW: 445.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	5.791E-01	15	K059	2 2 2 0 1	
2.915E-03	1.299E+00	c	D004	0 0 0 0 0	
1.016E-02	4.525E+00	h	D004	0 0 0 0 0	

4344. $C_{23}H_{27}N_3O_7$
Minocycline
Dynacin
Minocin
RN: 10118-90-8 **MP** (°C)**:**
MW: 457.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-01	5.200E+01	25	B191	1 0 0 0 1	neutral pH

4345. $C_{23}H_{28}ClN_3O_2S$
Thiopropazate
1-(2-Acetoxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine
RN: 84-06-0 **MP** (°C)**:**
MW: 446.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	8.920E-03	24	G022	2 0 1 1 1	

4346. $C_{23}H_{28}ClN_3O_5S$
Glyburide
HB 419
Glibenclamide
Diabeta
1-((*p*-(2-(5-Chloro-*o*-anisamido)ethyl)phenyl)-sulfonyl)-3-cyclohexylurea
RN: 10238-21-8 **MP** (°C)**:** 169
MW: 494.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-05	5.615E-03	22	M382	2 1 1 1 1	average of 2
6.275E-05	3.100E-02	25	G088	1 1 1 1 0	
1.000E-05	4.940E-03	25	Z410	0 0 0 0 0	EFG
8.097E-06	4.000E-03	27	H093	1 0 1 1 0	
2.024E-05	1.000E-02	ns	K444	0 0 0 0 0	

4347. $C_{23}H_{28}O_7$
Prednisone acetate
Pregna-1,4-diene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-
RN: 125-10-0 **MP** (°C)**:**
MW: 416.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.522E-05	2.300E-02	25	K003	2 1 1 1 1	

4348. $C_{23}H_{29}ClFN_3O_4$
Cisapride
4-Amino-5-chloro-*N*- [1-[3-(4-fluorophenoxy)propyl]-3-methoxy-4-piperidyl]-2-methoxy-benzamide
RN: 81098-60-4 **MP** (°C)**:**
MW: 465.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	9.319E-03	30	A417	0 0 0 0 0	pH 8.2
4.000E-04	1.864E-01	30	A417	0 0 0 0 0	pH 3.6

4349. $C_{23}H_{31}Cl_2NO_3$
Estramustine
Estradiol 3-[bis(2-chloroethyl)carbamate]
3-[bis(2-Chloroethyl)carbamate
RN: 2998-57-4 **MP** (°C)**:**
MW: 440.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.27E-06	~1.00E-03	30	L334	1 0 1 1 0	

4350. $C_{23}H_{31}FO_6$
9α-Fluorohydrocortisone acetate
Pregn-4-ene-3,20-dione, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β)-
RN: 514-36-3 **MP** (°C)**:**
MW: 422.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-04	5.400E-02	25	K021	1 2 2 2 1	

4351. $C_{23}H_{31}N_5O_4$
Benzoic acid, 3-[(dipropylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-71-1 **MP** (°C)**:**
MW: 441.53 **BP** (°C)**:** 674.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E-04	1.300E-01	21	B419	1 1 2 2 1	int

4352. $C_{23}H_{31}O_7$
Cortisone-21-hemi-succinate
RN: **MP** (°C)**:**
MW: 419.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.768E-04	2.000E-01	ns	E307	0 0 0 0 0	

4353. $C_{23}H_{32}O_2$
Medrogestone
Pregna-4,6-diene-3,20-dione, 6,17-dimethyl-
RN: 977-79-7 **MP** (°C)**:** 144
MW: 340.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.345E-06	1.820E-03	25	L033	1 0 2 1 2	

4354. $C_{23}H_{32}O_4$
Deoxycorticosterone acetate
Pregn-4-ene-3,20-dione, 21-(acetyloxy)-
RN: 56-47-3 **MP** (°C)**:** 156
MW: 372.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-05	4.000E-03	25	K003	2 1 1 1 1	

4355. $C_{23}H_{32}O_6$
Hydrocortisone acetate
Hydrocortisone-21-acetate
Cortisol acetate
Cortisol 21-acetate
RN: 50-03-3 **MP** (°C)**:** 223dec
MW: 404.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.486E-05	1.410E-02	25	C037	2 1 2 2 2	
1.555E-05	6.290E-03	25	H098	1 0 2 0 2	
1.555E-05	6.290E-03	25	H320	0 0 0 0 0	
1.550E-05	6.270E-03	25	H320	0 0 0 0 0	
2.472E-05	1.000E-02	25	K003	2 1 1 1 1	
3.461E-05	1.400E-02	25	K021	1 2 2 2 1	
2.472E-05	1.000E-02	25	M023	1 0 2 1 0	
2.472E-05	1.000E-02	ns	M169	0 0 0 0 1	
1.904E-05	7.700E-03	ns	N323	0 0 0 0 0	

4356. $C_{23}H_{34}O_3$
Testosterone butyrate
Androst-4-en-3-one, 17-(1-oxobutoxy)-, (17bet)-
RN: 3410-54-6 **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.406E-06	5.039E-04	25	J004	1 0 1 1 2	
1.403E-06	5.030E-04	ns	B057	0 2 1 1 2	

4357. $C_{23}H_{34}O_3$
5,6-Dehydroisoandrosterone butyrate
Androst-5-en-17-one, 3-(1-oxobutoxy)-, (3β)-
RN: 15253-51-7 **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.231E+00	4.413E+02	ns	B057	0 2 1 1 2	

4358. $C_{23}H_{34}O_3$
17-α-Methyltestosterone propionate
RN: **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.845E-06	1.020E-03	ns	B057	0 2 1 1 2	

4359. $C_{23}H_{34}O_4$
Digitoxigenin
Card-20(22)-enolide, 3,14-dihydroxy-, (3β,5β)-
RN: 143-62-4 **MP** (°C)**:**
MW: 374.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.124E-02	30	O321	0 0 0 0 0	

4360. $C_{23}H_{35}NOS$
5-Pregnene-20-one-3-spiro-2′-(1′,2′-thiazolidine)
RN: **MP** (°C)**:** 127–136
MW: 373.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.34E-05	~5.00E-03	ns	B199	0 0 0 0 0	

4361. $C_{23}H_{36}N_2O_2$
Finasteride
Proscar
RN: 98319-26-7 **MP** (°C)**:**
MW: 372.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-04	4.000E-02	amb	L434	0 0 0 0 0	

4362. $C_{23}H_{36}O_3$
Androstanolone butyrate
Androstan-3-one, 17-(1-oxobutoxy)-, (5α,17β)-
RN: 18069-66-4 **MP** (°C)**:**
MW: 360.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.220E-06	4.400E-04	ns	B057	0 2 1 1 2	

4363. $C_{23}H_{38}O_3$
Hexadecyl *p*-hydroxybenzoate
Hexadecyl 4-hydroxybenzoate
RN: 71067-09-9 **MP** (°C)**:**
MW: 362.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-03	3.789E-01	25	D081	1 2 2 1 2	

4364. $C_{23}H_{40}O_5$

4-Nonylphenol tetraethoxylate
p-Nonylphenol tetraethoxylate
RN: 7311-27-5 **MP** (°C)**:**
MW: 396.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-05	7.650E-03	20.5	A335	0 0 0 0 0	
1.930E-05	7.654E-03	20.5	A335	0 0 0 0 0	

4365. $C_{24}H_{12}$

Coronene
Coronen
RN: 191-07-1 **MP** (°C)**:** 438
MW: 300.36 **BP** (°C)**:** 525

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-09	1.406E-06	20	E009	1 0 0 1 2	
3.329E-10	1.000E-07	25	B319	2 0 1 2 1	
4.661E-10	1.400E-07	25	M064	1 1 2 2 1	
4.660E-10	1.400E-07	25	M342	1 0 1 1 2	

4366. $C_{24}H_{20}N_2$

N,*N*′-Diphenylbenzidine
RN: 531-91-9 **MP** (°C)**:** 247
MW: 336.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-07	6.000E-05	50	K068	1 0 2 2 0	buffer
1.783E-07	6.000E-05	rt	K068	0 0 2 2 0	buffer

4367. $C_{24}H_{22}N_2O_2$

G-3
p-Phenylpropylphenylbutazone
3,5-Pyrazolidinedione, 1,2-diphenyl-4-(3-phenylpropyl)-
RN: 32060-78-9 **MP** (°C)**:**
MW: 370.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.779E-04	1.400E-01	ns	B158	0 0 0 0 1	pH 7.0

4368. $C_{24}H_{26}N_2O_4$
Carvedilol
RN: 72956-09-3 **MP** (°C)**:**
MW: 406.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.492E-04	22.5	B440	0 0 0 0 0	
7.380E-05	3.000E-02	ns	S469	0 0 0 0 0	

4369. $C_{24}H_{26}N_4O_2$
Methyldiantipyrylmethane
MDAM
RN: 1606-56-0 **MP** (°C)**:**
MW: 402.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-03	4.498E-01	20	P054	0 0 0 0 0	

4370. $C_{24}H_{26}N_4S_2$
Methyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-ethylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-70-5 **MP** (°C)**:** 229
MW: 434.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.173E-01	ns	D087	0 2 0 0 1	

4371. $C_{24}H_{27}BrN_6O_{10}$
C.I. Disperse blue 79
2′-Acetylamino-4′-[bis(acetoxyethyl)amino]-6-bromo-2,4-dinitro-5′-ethoxyazobenzene
RN: 12239-34-8 **MP** (°C)**:** 146
MW: 639.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-09	6.394E-07	25	B333	0 0 0 0 0	

4372. $C_{24}H_{27}N$
Prenylamine
N-(3,3-Diphenylpropyl)-α-methylphenylethylamine
RN: 390-64-7 **MP** (°C)**:** 36.5
MW: 329.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.517E-04	5.000E-02	37	C054	2 0 2 1 0	

4373. $C_{24}H_{29}N_5O_3$
Valsartan
(2*S*)-3-Methyl-2-[pentanoyl-[[4-[2-(2H-tetrazol-5-yl)phenyl]phenyl]methyl]amino]butanoic acid
RN: 137862-53-4 **MP** (°C)**:**
MW: 435.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.951E-04	8.499E-02	25	C431	0 0 0 0 0	

4374. $C_{24}H_{30}F_2O_6$
Fluocinolone acetonide
6α,9α-Difluoro-16α hydroxyprednisolone-16,17-acetonide
6α,9α-Difluoro-16α,17α-isopropylidenedioxy-1,4-pregnadiene-3,20-dione
RN: 67-73-2 **MP** (°C)**:** 260.5
MW: 452.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-04	1.080E-01	25	K021	1 2 2 2 1	
4.641E-05	2.100E-02	25	O001	2 0 2 2 2	
2.210E-04	1.000E-01	25	P008	0 0 0 0 0	EFG

4375. $C_{24}H_{31}ClO_7$
Loteprednol etabonate
Lenoxin
Androsta-1,4-diene-17-carboxylic acid
17-[(Ethoxycarbonyl)oxy]-11-hydroxy-3-oxo-chloromethyl ester, (11b,17a)-
RN: 82034-46-6 **MP** (°C)**:**
MW: 466.96 **BP** (°C)**:** 600.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.14E-06	<1.00E-03	23	B409	1 0 0 0 1	

4376. $C_{24}H_{31}FO_5S$
Timobesone acetate
17-β-Methythiocarbonyl-9α-fluoro-11β
RN: 79578-14-6 **MP** (°C)**:**
MW: 450.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	2.703E+00	25	O318	0 0 0 0 0	

4377. $C_{24}H_{31}FO_6$

Triamcinolone acetonide
9α-Fluoro-16α-hydroxyprednisolone acetonide
Triamcinolone 16α,17-acetonide
Aristoderm
Adcortyl-A

RN: 76-25-5 **MP** (°C)**:** 293
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.205E-05	4.000E-02	23	F025	1 0 0 0 0	
9.436E-05	4.100E-02	25	K021	1 2 2 2 1	
6.076E-04	2.640E-01	25	L009	1 0 0 1 1	
4.833E-05	2.100E-02	28	B055	2 0 2 2 2	
4.027E-05	1.750E-02	28	B056	1 2 1 1 2	
5.869E-05	2.550E-02	37	B055	2 0 2 2 2	
4.764E-05	2.070E-02	37	B056	1 2 1 1 2	
9.205E-05	4.000E-02	37	F025	1 0 0 0 0	
7.733E-05	3.360E-02	50	B055	2 0 2 2 2	
6.099E-05	2.650E-02	50	B056	1 2 1 1 2	
2.532E-04	1.100E-01	amb	L434	0 0 0 0 0	

4378. $C_{24}H_{31}FO_6$

Betamethasone acetate
Betamethasone-17-acetate
9α-Fluoro-16β-methylprednisolone-21-acetate

RN: 987-24-6 **MP** (°C)**:** 200dec
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.904E-05	3.000E-02	25	K003	2 1 1 1 1	

4379. $C_{24}H_{31}FO_6$

Dexamethasone acetate
Dexamethasone-17-acetate
Dexamethasone acetate

RN: 1177-87-3 **MP** (°C)**:** 263
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.992E-05	1.300E-02	25	K003	2 1 1 1 1	
6.214E-05	2.700E-02	37	D026	0 0 0 0 0	

4380. $C_{24}H_{31}NO_4$

Drotaverine
1-(3,4-Diethoxybenzylidene)-6,7-diethoxy-1,2,3,4-tetrahydroisoquinoline
RN: 14009-24-6 **MP** (°C)**:**
MW: 397.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-02	1.375E+01	37	C054	2 0 2 1 2	

4381. $C_{24}H_{32}N_2O_9$

Enalapril maleate
L-Proline, 1-[*N*-[1-(ethoxycarbonyl)-3-phenylpropyl]-L-alanyl]-,
(*S*)-1-(*N*-(1-(Ethoxycarbonyl)-3-phenylpropyl)-L-alanyl)-L-proline, (Z)-2-butenedioate salt
RN: 76095-16-4 **MP** (°C)**:**
MW: 492.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.264E-02	2.100E+01	25	A412	1 0 2 2 1	int

4382. $C_{24}H_{32}O_4$

Ethynodiol diacetate
Ovulen-50
RN: 297-76-7 **MP** (°C)**:** 126
MW: 384.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.641E-06	1.400E-03	25	L027	1 0 0 0 2	

4383. $C_{24}H_{32}O_4S$

Spironolactone
17-Hydroxy-7α-mercapto-3-oxo-17α-pregn-4-ene-21-carboxylic acid γ-lactone acetate
Spiractin
RN: 52-01-7 **MP** (°C)**:** 134
MW: 416.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-06	2.999E-03	25	A348	0 0 0 0 0	
5.281E-05	2.200E-02	25	C037	2 1 2 2 2	
5.281E-05	2.200E-02	25	G084	2 0 2 2 1	
4.801E-05	2.000E-02	25	G095	2 1 2 2 1	
6.649E-05	2.770E-02	37	K092	2 0 0 1 2	
2.400E-05	1.000E-02	ns	K444	0 0 0 0 0	

4384. $C_{24}H_{32}O_5$
7-Carboxylic acid methyl ester canrenone
RN: **MP** (°C)**:**
MW: 400.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	7.850E-02	37	C004	0 0 0 0 0	EFG

4385. $C_{24}H_{32}O_6$
Cortisone 17-propionate
Pregn-4-ene-3,11,20-trione, 21-hydroxy-17-(1-oxopropoxy)-
RN: 136370-32-6 **MP** (°C)**:**
MW: 416.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.921E-05	8.000E-03	25	M023	1 0 2 1 0	

4386. $C_{24}H_{33}FO_6$
Flurandrenolone
Fludroxycortide
6-Fluoro-16α-hydroxyhydrocortisone-16,17-acetonide
RN: 1524-88-5 **MP** (°C)**:**
MW: 436.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.758E-04	2.950E-01	25	K021	1 2 2 2 1	

4387. $C_{24}H_{34}N_2O$
Bepridil
1-Isobutoxy-2-pyrrolidino-3-*N*-benzylanilino-propane
Bepadin
RN: 64706-54-3 **MP** (°C)**:**
MW: 366.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.027E-02	7.430E+00	37	N032	1 0 1 1 2	

4388. $C_{24}H_{34}N_2O_3$
Lysine estrone ester
RN: **MP** (°C)**:**
MW: 398.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	1.260E+02	ns	A074	0 0 0 0 0	EFG

4389. $C_{24}H_{34}O_5$

Dehydrocholic acid
3,7,12-Trioxo-5β-cholanic acid
RN: 81-23-2 **MP** (°C)**:** 237
MW: 402.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-04	1.800E-01	15	G081	1 0 1 1 1	
1.615E-04	6.500E-02	30	O321	0 0 0 0 0	
1.600E-04	6.441E-02	30	O321	0 0 0 0 0	

4390. $C_{24}H_{34}O_6$

Hydrocortisone propionate
Hydrocortisone-21-propionate
RN: 6677-98-1 **MP** (°C)**:**
MW: 418.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.772E-05	1.160E-02	25	H098	1 0 2 0 2	
2.772E-05	1.160E-02	25	H320	0 0 0 0 0	
2.770E-05	1.159E-02	25	H320	0 0 0 0 0	

4391. $C_{24}H_{36}O_3$

Testosterone valerate
Androst-4-en-3-one, 17-[(1-oxopentyl)oxy]-, (17β)-
Testosterone 17-valerate
RN: 3129-43-9 **MP** (°C)**:**
MW: 372.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.778E-07	2.898E-04	25	J004	1 0 1 1 2	
7.811E-07	2.910E-04	ns	B057	0 2 1 1 2	

4392. $C_{24}H_{36}O_3$

5,6-Dehydroisoandrosterone valerate
Androst-5-en-17-one, 3-[(1-oxopentyl)oxy]-, (3β)-
RN: 7642-68-4 **MP** (°C)**:**
MW: 372.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.061E-05	7.680E-03	ns	B057	0 2 1 1 2	

4393. $C_{24}H_{38}O_3$
Androstanolone valerate
Androstan-3-one, 17-[(1-oxopentyl)oxy]-, (5α,17β)-
RN: 26271-72-7 **MP** (°C)**:**
MW: 374.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.143E-07	3.050E-04	ns	B057	0 2 1 1 2	

4394. $C_{24}H_{38}O_4$
Di-2-ethylhexyl isophthalate
D-(2-Ethylhexyl) isophthalate
Dioctyl isophthalate
RN: 137-89-3 **MP** (°C)**:**
MW: 390.57 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.816E-08	1.100E-05	24	H116	2 1 0 0 2	

4395. $C_{24}H_{38}O_4$
Octyl phthalate
Di(2-ethylhexyl)phthalate
Di-(2-ethylhexyl)-phthalate
Di-*sec*-octyl phthalate
bis(2-Ethylhexyl) phthalate
bis-(2-Ethylhexyl) 1,2-benzenedicarboxylate
RN: 117-81-7 **MP** (°C)**:** –50
MW: 390.57 **BP** (°C)**:** 386.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	9.999E-02	20	F070	1 0 0 0 1	*sic*
1.050E-07	4.101E-05	20	L300	2 1 0 2 2	
1.536E-06	6.000E-04	22.5	G301	0 0 0 0 0	
7.297E-07	2.850E-04	24	H116	2 1 0 0 2	
6.913E-07	2.700E-04	25	D336	0 0 0 0 0	
1.280E-06	5.000E-04	25	F067	1 0 2 2 0	

4396. $C_{24}H_{38}O_4$
Apocholic acid
RN: 641-81-6 **MP** (°C)**:** 175.5
MW: 390.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-03	8.000E-01	15	G081	1 0 1 1 0	

4397. $C_{24}H_{38}O_4$
bis(Tereoctyl) phthalate
RN: **MP** (°C)**:**
MW: 390.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.633E-08	2.200E-05	25	D336	0 0 0 0 0	

4398. $C_{24}H_{38}O_4$
bis(Isooctyl) phthalate
Diisooctyl phthalate
1,2-Benzenedicarboxylic acid diisooctyl ester
RN: 27554-26-3 **MP** (°C)**:** -4
MW: 390.57 **BP** (°C)**:** 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E-07	4.000E-05	25	D336	0 0 0 0 0	

4399. $C_{24}H_{38}O_4$
bis(*n*-Octyl) phthalate
Di-*n*-octyl phthalate
1,2-Benzenedicarboxylic acid
RN: 117-84-0 **MP** (°C)**:** –25
MW: 390.57 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-08	2.000E-05	25	D336	0 0 0 0 0	

4400. $C_{24}H_{39}NO_3$
Acetaminophen palmitate
Acetaminophen hexadecanoate
RN: 54942-40-4 **MP** (°C)**:** 117
MW: 389.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.283E-05	5.000E-03	25	B010	1 1 1 1 0	

4401. $C_{24}H_{40}N_8O_4$
Dypyridamole
2,6-bis(Diethanolamino)-4,8-dipiperidinopyrimido-[5,4-d]pyrimidin
Dipridacot
Dipryridamole
Persantin
Dipyridamol
RN: 58-32-2 **MP** (°C)**:**
MW: 504.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.649E-06	8.320E-04	22.5	B440	0 0 0 0 0	
7.000E-05	3.532E-02	30	A417	0 0 0 0 0	pH 5.2
3.200E-03	1.615E+00	30	A417	0 0 0 0 0	pH 3.7

4402. $C_{24}H_{40}O_3$
3β-Hydroxy-5β-cholanoic acid
7α-Hydroxy-5β-cholanoic acid
RN: **MP** (°C)**:**
MW: 376.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	6.779E-05	10	F307	1 2 2 2 2	pH 3.0
4.400E-07	1.657E-04	10	F307	1 2 2 2 2	pH 3.0
5.200E-07	1.958E-04	15	F307	1 2 2 2 2	pH 3.0
2.200E-07	8.285E-05	15	F307	1 2 2 2 2	pH 3.0
2.400E-07	9.038E-05	20	F307	1 2 2 2 2	pH 3.0
6.500E-07	2.448E-04	20	F307	1 2 2 2 2	pH 3.0
2.800E-07	1.054E-04	25	F307	1 2 2 2 2	pH 3.0
7.900E-07	2.975E-04	25	F307	1 2 2 2 2	pH 3.0
3.500E-07	1.318E-04	30	F307	1 2 2 2 2	pH 3.0
9.700E-07	3.653E-04	30	F307	1 2 2 2 2	pH 3.0
5.300E-07	1.996E-04	35	F307	1 2 2 2 2	pH 3.0
1.190E-06	4.481E-04	35	F307	1 2 2 2 2	pH 3.0
8.200E-07	3.088E-04	40	F307	1 2 2 2 2	pH 3.0
1.490E-06	5.611E-04	40	F307	1 2 2 2 2	pH 3.0
1.770E-06	6.666E-04	45	F307	1 2 2 2 2	pH 3.0
1.280E-06	4.820E-04	45	F307	1 2 2 2 2	pH 3.0
1.500E-06	5.649E-04	50	F307	1 2 2 2 2	pH 3.0
2.150E-06	8.097E-04	50	F307	1 2 2 2 2	pH 3.0

4403. $C_{24}H_{40}O_3$

Lithocholic acid
3α-Hydroxy-5β-cholan-24-oic acid
3α-Hydroxycholanic acid
RN: 434-13-9 **MP** (°C)**:** 184
MW: 376.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.431E-05	10	F307	1 2 2 2 2	pH 3.0
4.000E-08	1.506E-05	15	F307	1 2 2 2 2	pH 3.0
4.600E-08	1.732E-05	20	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	20	I012	1 2 2 1 0	pH 2.4
5.000E-08	1.883E-05	25	F307	1 2 2 2 2	pH 3.0
6.000E-08	2.260E-05	30	F307	1 2 2 2 2	pH 3.0
7.500E-08	2.824E-05	35	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	37	I012	1 2 2 1 0	pH 2.4
1.000E-07	3.766E-05	40	F307	1 2 2 2 2	pH 3.0
1.100E-07	4.142E-05	45	F307	1 2 2 2 2	pH 3.0
1.400E-07	5.272E-05	50	F307	1 2 2 2 2	pH 3.0

4404. $C_{24}H_{40}O_4$

Hyodeoxycholic acid
3α,6β-Dihydroxy-5α-cholanoic acid
RN: 83-49-8 **MP** (°C)**:** 198
MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.926E-03	10	F307	1 2 2 2 2	pH 3.0
1.200E-05	4.711E-03	15	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	20	F307	1 2 2 2 2	pH 3.0
1.500E-05	5.889E-03	25	F307	1 2 2 2 2	pH 3.0
1.700E-05	6.674E-03	30	F307	1 2 2 2 2	pH 3.0
1.800E-05	7.067E-03	35	F307	1 2 2 2 2	pH 3.0
2.000E-05	7.852E-03	40	F307	1 2 2 2 2	pH 3.0
2.200E-05	8.637E-03	45	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	50	F307	1 2 2 2 2	pH 3.0

4405. $C_{24}H_{40}O_4$

Deoxycholic acid
Cholan-24-oic acid, 3,12-dihydroxy-, (3α,5β,12α)-
3α,12α-Dihydroxy-5β-cholanoic acid
RN: 83-44-3 **MP** (°C)**:** 176
MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-05	9.422E-03	10	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	15	F307	1 2 2 2 2	pH 3.0
6.113E-04	2.400E-01	15	G081	1 0 1 1 1	

(*continued*)

4405. $C_{24}H_{40}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.093E-04	2.000E-01	20	D041	1 0 0 0 0	
2.700E-05	1.060E-02	20	F307	1 2 2 2 2	pH 3.0
1.110E-04	4.358E-02	20	I012	1 2 2 1 2	pH 2.4
2.800E-05	1.099E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
2.900E-05	1.138E-02	35	F307	1 2 2 2 2	pH 3.0
1.140E-04	4.475E-02	37	I012	1 2 2 1 2	pH 2.4
2.900E-05	1.138E-02	40	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	45	F307	1 2 2 2 2	pH 3.0
3.200E-05	1.256E-02	50	F307	1 2 2 2 2	pH 3.0

4406. $C_{24}H_{40}O_4$

Chenodeoxycholic acid

CDCA

RN: 474-25-9 **MP** (°C)**:** 119

MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	9.815E-03	10	F307	1 2 2 2 2	pH 3.0
2.500E-05	9.815E-03	15	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	20	F307	1 2 2 2 2	pH 3.0
2.290E-04	8.990E-02	20	I012	1 2 2 1 2	pH 2.4
2.700E-05	1.060E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	35	F307	1 2 2 2 2	pH 3.0
2.560E-04	1.005E-01	37	I008	1 0 0 1 2	
2.560E-04	1.005E-01	37	I012	1 2 2 1 2	pH 2.4
3.150E-05	1.237E-02	40	F307	1 2 2 2 2	pH 3.0
3.400E-05	1.335E-02	45	F307	1 2 2 2 2	pH 3.0
3.600E-05	1.413E-02	50	F307	1 2 2 2 2	pH 3.0
2.291E-04	8.994E-02	ns	R427	0 0 0 0 0	

4407. $C_{24}H_{40}O_4$

Ursodeoxycholic acid

UDCA

RN: 128-13-2 **MP** (°C)**:** 203

MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.748E-03	10	F307	1 2 2 2 2	pH 3.0
7.500E-06	2.944E-03	15	F307	1 2 2 2 2	pH 3.0
8.000E-06	3.141E-03	20	F307	1 2 2 2 2	pH 3.0
5.100E-05	2.002E-02	20	I012	1 2 2 1 1	pH 2.4
9.000E-06	3.533E-03	25	F307	1 2 2 2 2	pH 3.0
1.000E-05	3.926E-03	30	F307	1 2 2 2 2	pH 3.0

(*continued*)

4407. $C_{24}H_{40}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-05	4.515E-03	35	F307	1 2 2 2 2	pH 3.0
5.300E-05	2.081E-02	37	I008	1 0 0 1 1	
5.300E-05	2.081E-02	37	I012	1 2 2 1 1	pH 2.4
1.200E-05	4.711E-03	40	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	45	F307	1 2 2 2 2	pH 3.0
1.400E-05	5.496E-03	50	F307	1 2 2 2 2	pH 3.0
8.556E-04	3.359E-01	ns	K446	0 0 0 0 0	

4408. $C_{24}H_{40}O_5$

3α, 6α, 7α -Trihydroxy-5β-cholanate

RN: **MP** (°C)**:**

MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-05	1.512E-02	10	F307	1 2 2 2 2	pH 3.0
3.800E-05	1.553E-02	15	F307	1 2 2 2 2	pH 3.0
4.100E-05	1.675E-02	20	F307	1 2 2 2 2	pH 3.0
4.500E-05	1.839E-02	25	F307	1 2 2 2 2	pH 3.0
5.500E-05	2.247E-02	30	F307	1 2 2 2 2	pH 3.0
6.900E-05	2.819E-02	35	F307	1 2 2 2 2	pH 3.0
8.600E-05	3.514E-02	40	F307	1 2 2 2 2	pH 3.0
1.160E-04	4.740E-02	45	F307	1 2 2 2 2	pH 3.0
1.600E-04	6.537E-02	50	F307	1 2 2 2 2	pH 3.0

4409. $C_{24}H_{40}O_5$

Ursocholic acid

3α,7β,12α-Trihydroxy-5β-cholanoic acid

RN: 2955-27-3 **MP** (°C)**:**

MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-03	6.496E-01	10	F307	1 2 2 2 2	pH 3.0
1.610E-03	6.578E-01	15	F307	1 2 2 2 2	pH 3.0
1.640E-03	6.701E-01	20	F307	1 2 2 2 2	pH 3.0
1.670E-03	6.823E-01	25	F307	1 2 2 2 2	pH 3.0
1.710E-03	6.987E-01	30	F307	1 2 2 2 2	pH 3.0
1.762E-03	7.199E-01	35	F307	1 2 2 2 2	pH 3.0
1.828E-03	7.469E-01	40	F307	1 2 2 2 2	pH 3.0
1.872E-03	7.649E-01	45	F307	1 2 2 2 2	pH 3.0
2.000E-03	8.172E-01	50	F307	1 2 2 2 2	pH 3.0

4410. $C_{24}H_{40}O_5$
Cholic acid
Cholsaeure
RN: 81-25-4 **MP** (°C)**:** 198
MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-04	9.030E-02	10	F307	1 2 2 2 2	pH 3.0
6.486E-04	2.650E-01	15	F300	1 0 0 0 0	
2.140E-04	8.744E-02	15	F307	1 2 2 2 2	pH 3.0
6.853E-04	2.800E-01	15	G081	1 0 1 1 1	
6.851E-04	2.799E-01	20	D041	1 0 0 0 1	
2.247E-04	9.180E-02	20	E008	1 0 2 0 2	average of 3
2.200E-04	8.989E-02	20	F307	1 2 2 2 2	pH 3.0
4.280E-04	1.749E-01	20	I012	1 2 2 1 2	pH 2.4
2.350E-04	9.602E-02	25	F307	1 2 2 2 2	pH 3.0
2.670E-04	1.091E-01	30	F307	1 2 2 2 2	pH 3.0
3.240E-04	1.324E-01	35	F307	1 2 2 2 2	pH 3.0
4.600E-04	1.879E-01	37	I012	1 2 2 1 2	pH 2.4
3.830E-04	1.565E-01	40	F307	1 2 2 2 2	pH 3.0
4.830E-04	1.973E-01	45	F307	1 2 2 2 2	pH 3.0
6.390E-04	2.611E-01	50	F307	1 2 2 2 2	pH 3.0

4411. $C_{24}H_{50}$
Tetracosane
n-Tetracosane
Alkane C(24)
RN: 646-31-1 **MP** (°C)**:** 54
MW: 338.67 **BP** (°C)**:** 391.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.264E-02	4.282E+00	321	S355	1 1 1 2 0	EFG
8.878E-02	3.007E+01	369	S355	1 1 1 2 0	EFG

4412. $C_{24}H_{51}OP$
tri-*n*-Octylphosphine oxide
TOPO
Trioctylphosphine oxide
RN: 78-50-2 **MP** (°C)**:**
MW: 386.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-06	2.800E-03	0	O002	2 0 2 2 1	
3.880E-06	1.500E-03	25	O002	2 0 2 2 1	

4413. $C_{24}H_{51}O_3P$
Dibutyl hexadecyl phosphonate
Phosphonic acid, hexadecyl-, dibutyl ester
RN: 84869-93-2 **MP** (°C)**:**
MW: 418.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.78E-04	<2.00E-01	25	B070	1 2 0 1 0	

4414. $C_{24}H_{51}O_4P$
tris-(2-Ethylhexyl) phosphate
Disflamoll TOF
TEHP
Flexol TOF
RN: 78-42-2 **MP** (°C)**:**
MW: 434.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-06	6.000E-04	24	H116	2 1 0 0 2	

4415. $C_{24}H_{54}OSn_2$
bis(Tributyltin) oxide
6-Oxa-5,7-distannaundecane, 5,5,7,7-tetrabutyl-
RN: 56-35-9 **MP** (°C)**:**
MW: 596.08 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E-04	1.000E-01	rt	M161	0 0 0 0 2	

4416. $C_{25}H_{22}O_{10}$
Silybin
Silibinin
Silybum substance E6
Silymarin I
RN: 22888-70-6 **MP** (°C)**:**
MW: 482.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.788E-05	4.240E-02	19.99	B439	0 0 0 0 0	
1.119E-04	5.400E-02	24.99	B439	0 0 0 0 0	
1.432E-04	6.910E-02	29.99	B439	0 0 0 0 0	
1.726E-04	8.329E-02	34.99	B439	0 0 0 0 0	
2.066E-04	9.969E-02	39.99	B439	0 0 0 0 0	

4417. $C_{25}H_{24}F_6N_4$
Hydramethylnon
Amdro
Comat
Amidinohydrazone;
Wipeout
Tetrahydro-5,5-dimethyl-2(1H)-pyrimidinone[3-[4-(trifluoromethyl)phenyl]-1-[2-[4-(trifluoromethyl)phenyl]ethenyl]-2-propenylidene]hydrazone
RN: 67485-29-4 **MP** (°C)**:** 185–190
MW: 494.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-08	5.945E-06	ns	R427	0 0 0 0 0	

4418. $C_{25}H_{24}N_2O_2S$
G-8
o,p-Dimethylphenylthioethylphenylbutazone
3,5-Pyrazolidinedione, 1,2-diphenyl-4-[2-(2,4-xylylthio)ethyl]-
RN: 102892-46-6 **MP** (°C)**:**
MW: 416.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-04	1.300E-01	ns	B158	0 0 0 0 1	pH 7.0

4419. $C_{25}H_{28}N_4O_2$
Ethyldiantipyrylmethane
EDAM
RN: 61358-28-9 **MP** (°C)**:**
MW: 416.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.601E-04	1.500E-01	20	P054	0 0 0 0 0	

4420. $C_{25}H_{28}O_3$
Estradiol benzoate
Estradiol monobenzoate
7β-Estradiol-3-benzoate
RN: 50-50-0 **MP** (°C)**:** 190
MW: 376.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-06	4.000E-04	25	K003	2 1 1 1 1	
1.072E-06	4.034E-04	ns	R427	0 0 0 0 0	

4421. $C_{25}H_{28}O_3$
Ethofenprox
1-((2-(4-Ethoxyphenyl)-2-methylpropoxy)methyl)-3-phenoxybenzene
Etofenprox
Zoecon
MTI-500
Trebon
RN: 80844-07-1 **MP** (°C)**:**
MW: 376.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-09	9.457E-07	ns	R427	0 0 0 0 0	

4422. $C_{25}H_{29}I_2NO_3$
Amiodarone
Cordarone
Aratac
RN: 1951-25-3 **MP** (°C)**:**
MW: 645.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.72E-08	<4.34E-05	22.5	B440	0 0 0 0 0	
1.110E-03	7.164E-01	25	B337	2 2 2 1 2	

4423. $C_{25}H_{31}FO_8$
Triamcinolone 16, 21-diacetate
Pregna-1,4-diene-3,20-dione, 16,21-bis(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β,16apha)-
RN: 67-78-7 **MP** (°C)**:** 235
MW: 478.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-04	4.800E-02	25	F026	0 0 0 0 0	

4424. $C_{25}H_{31}NO_2$
3-Hydroxy-17β-{[(1-methyl-1,4-dihydropyridin-3-yl)-carbonyl]oxy}-estra-1,3,5(10)-triene
RN: **MP** (°C)**:**
MW: 377.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-07	6.580E-05	25	B366	0 0 0 0 0	

4425. $C_{25}H_{34}O_3$
Norethindrone dimethylpropionate
19-Norpregn-4-en-20-yn-3-one, 17-(2,2-dimethyl-1-oxopropoxy)-, (17α)-
RN: 65445-09-2 **MP** (°C)**:**
MW: 382.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.894E-08	3.020E-05	25	L078	1 0 1 2 2	

4426. $C_{25}H_{34}O_6$
Budesonide
16,17-Butylidenebis(oxy)-11-,21-dihydroxypregna-1,4-diene-3,20-dione
Rhinocort
RN: 51333-22-3 **MP** (°C)**:**
MW: 430.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	2.153E-02	ns	F327	0 0 1 2 2	

4427. $C_{25}H_{34}O_9$
6-(1,3-Dihydro-7-acetate-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic solketal ester
RN: **MP** (°C)**:**
MW: 478.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-05	9.000E-03	25	L333	1 1 1 1 0	

4428. $C_{25}H_{35}N_5O_4$
Benzoic acid, 3-[(dibutylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-73-3 **MP** (°C)**:**
MW: 469.59 **BP** (°C)**:** 688.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-05	6.000E-03	21	B419	1 1 2 2 1	int

4429. $C_{25}H_{36}N_4O_7$
Nonyloxycarbonyl-mitomycin C
2′-(2-Hexanoyl-2-pentanyl-acetyl)-6-methoxypurine arabinoside
RN: **MP** (°C)**:**
MW: 504.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	1.261E-04	25	M316	1 1 1 1 2	
2.020E-03	1.019E+00	37	C348	0 0 0 0 0	pH 7.00

4430. $C_{25}H_{36}O_6$
Hydrocortisone butyrate
Hydrocortisone-21-butyrate
11,17-Dihydroxy-21-(1-oxobutoxy)-pregn-4-ene-3,20-dione
RN: 6677-99-2 **MP** (°C)**:**
MW: 432.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-05	7.730E-03	25	H098	1 0 2 0 2	
1.787E-05	7.730E-03	25	H320	0 0 0 0 0	
1.780E-05	7.700E-03	25	H320	0 0 0 0 0	

4431. $C_{25}H_{36}O_7$
5,16-β-Dihydroxy-6-β-methyl-3,11-dioxo-5-α-pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester cycl
RN: **MP** (°C)**:**
MW: 448.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.672E-04	7.500E-02	ns	K029	0 0 2 1 1	

4432. $C_{25}H_{40}O_3Si_2$
Norethindrone pentamethyldisiloxyl ether
RN: **MP** (°C)**:**
MW: 444.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.301E-07	1.023E-04	25	L078	1 0 1 2 2	

4433. $C_{25}H_{42}O_3$
Octadecyl-*p*-hydroxybenzoate
RN: 71067-10-2 **MP** (°C)**:**
MW: 390.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.343E-04	3.259E-01	25	D081	1 2 2 1 2	

4434. $C_{25}H_{44}$
Nonadecylbenzene
1-Phenylnonadecane
RN: 29136-19-4 **MP** (°C)**:**
MW: 344.63 **BP** (°C)**:** 419

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-02	5.272E+00	328	S355	1 1 1 2 0	EFG
2.396E-01	8.257E+01	363	S355	1 1 1 2 0	EFG

4435. $C_{25}H_{44}O_6$
4-Nonylphenol pentaethoxylate
RN: 20636-48-0 **MP** (°C)**:**
MW: 440.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E-05	9.480E-03	20.5	A335	0 0 0 0 0	
2.150E-05	9.473E-03	20.5	A335	0 0 0 0 0	

4436. $C_{25}H_{48}O_4$
Dioctyl azelate
Di(2-ethylhexyl) azelate
RN: 103-24-2 **MP** (°C)**:**
MW: 412.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.423E-07	1.000E-04	25	F067	1 0 2 2 0	

4437. $C_{25}H_{54}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)methane
HDPM
RN: 2785-33-3 **MP** (°C)**:**
MW: 448.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	6.400E-02	0	O002	2 0 2 2 0	EFG
8.849E-05	3.970E-02	25	O002	2 0 2 2 1	average of 2
6.241E-05	2.800E-02	35	O002	2 0 2 2 0	EFG
4.458E-05	2.000E-02	40	O002	2 0 2 2 0	EFG
3.377E-03	1.515E+00	45	O002	2 0 2 2 0	EFG

4438. $C_{26}H_{18}N_2O_4$
Samaron violet
Mowilith red 3B(IG)
RN: 6408-72-6 **MP** (°C)**:**
MW: 422.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	1.267E-03	98.59	M180	0 0 2 2 0	EFG
4.000E-06	1.690E-03	109.98	M180	0 0 2 1 0	EFG
4.500E-06	1.901E-03	120.54	M180	0 0 2 2 0	EFG
6.000E-06	2.535E-03	133.34	M180	0 0 2 2 0	EFG
8.000E-06	3.380E-03	141.78	M180	0 0 2 2 0	EFG

4439. $C_{26}H_{20}N_2O_8S_2$
1,5-Anthraquinone disulfonic acid anilide
RN: **MP** (°C)**:**
MW: 552.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.210E-03	3.984E+00	18	F047	1 2 1 1 1	

4440. $C_{26}H_{20}N_2O_8S_2$
1,8-Anthraquinone disulfonic acid anilide
RN: **MP** (°C)**:**
MW: 552.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.209E-02	2.326E+01	18	F047	1 2 1 1 1	

4441. $C_{26}H_{28}Cl_2N_4O_4$
Ketoconazole
(±)-*cis*-1-Acetyl-4-(4-[(2-[2,4-dichlorophenyl]-2-[1H-imidazol-1-ylmethyl]-1,3-dioxolan-4-yl)-methoxy]phenyl)piperazine
RN: 65277-42-1 **MP** (°C)**:**
MW: 531.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.505E-04	8.000E-02	37	C323	0 0 0 0 0	EFG
1.882E-05	1.000E-02	amb	L434	0 0 0 0 0	

4442. $C_{26}H_{28}N_2$
Cinnarizine
Stugeron
RN: 298-57-7 **MP** (°C)**:**
MW: 368.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.035E-03	7.500E-01	ns	B155	0 0 1 1 0	EFG, pH 3.0

4443. $C_{26}H_{28}N_4O_2$
Propyldiantipyrylmethane
PDAM
RN: 1461-17-2 **MP** (°C)**:**
MW: 428.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	6.000E-02	20	P054	0 0 0 0 0	

4444. $C_{26}H_{29}NO$
Tamoxifen
Genox
Kessar
Nolvadex
(Z)-2-[4-(1,2-Diphenyl-1-butenyl)phenoxy]-*N*,*N*-dimethylethanamine
Tamoxen
RN: 10540-29-1 **MP** (°C)**:**
MW: 371.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.550E+00	2.805E+03	25	B443	0 0 0 0 0	extrapolated
		amb	L434	0 0 0 0 0	

4445. $C_{26}H_{30}Cl_2F_3NO$

Halofantrine
1-(1,3-Dichloro-6-trifluoromethyl-9-phenanthryl)-3-di(*n*-butyl)aminopropanol
RN: 69756-53-2 **MP** (°C)**:**
MW: 500.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-06	5.900E-04	37	A423	0 0 0 0 0	

4446. $C_{26}H_{30}N_4O_2$

Isopropyldiantipyrylmethane
IPDAM
RN: 15536-49-9 **MP** (°C)**:**
MW: 430.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-04	2.000E-01	20	P054	0 0 0 0 0	

4447. $C_{26}H_{30}N_4S_2$

Propyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-butylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 57094-83-4 **MP** (°C)**:** 222
MW: 462.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	1.110E-01	ns	D087	0 2 0 0 1	

4448. $C_{26}H_{31}ClN_2O_8S$

Amlodipine
Amlodipine besylate
Norvasc
(*RS*)-3-Ethyl-5-methyl-2-(2-aminoethoxymethyl)-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridinedicarboxylate benzenesulfonate
RN: 88150-42-9 **MP** (°C)**:**
MW: 567.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.76E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4449. $C_{26}H_{32}F_2O_7$
Diflorasone diacetate
U-34865
RN: 33564-31-7 **MP** (°C)**:**
MW: 494.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.314E-05	6.500E-03	25	F003	0 0 0 0 0	
1.254E-05	6.200E-03	37	F003	0 0 0 0 0	
2.629E-05	1.300E-02	50	F003	0 0 0 0 0	

4450. $C_{26}H_{32}F_2O_7$
Fluocinolide
Fluocinonide
Fluocinolone acetonide acetate
RN: 356-12-7 **MP** (°C)**:**
MW: 494.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-06	5.300E-04	25	O001	2 0 2 2 2	
2.022E-05	1.000E-02	25	P008	0 0 0 0 0	EFG

4451. $C_{26}H_{32}O_3$
Testosterone benzoate
Androst-4-en-3-one, 17-(benzoyloxy)-, (17β)-
RN: 2088-71-3 **MP** (°C)**:**
MW: 392.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.312E-05	1.300E-02	25	L342	1 0 1 1 2	

4452. $C_{26}H_{36}O_3$
Norethisterone heptanoate
RN: **MP** (°C)**:**
MW: 396.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.521E-07	6.030E-05	25	E301	1 0 1 1 2	

4453. $C_{26}H_{36}O_6$
Prednisolone 21-trimethylacetate
Prednisolone acetate
RN: 52-21-1 **MP** (°C)**:** 233
MW: 444.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-05	1.160E-02	25	C037	2 1 2 2 2	
6.298E-05	2.800E-02	25	K021	1 2 2 2 1	
2.699E-05	1.200E-02	ns	N302	0 2 1 2 1	

4454. $C_{26}H_{37}FO_5$
Dexamethasone TBA
RN: **MP** (°C)**:**
MW: 448.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.229E-05	1.000E-02	37	D026	0 0 0 0 0	

4455. $C_{26}H_{38}NO_8$
Glucosamine testosterone
17-β-(4-Androsten-3-one)-*N*-2-(2-desoxyglucosyl)
RN: **MP** (°C)**:** 185–190
MW: 492.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	6.560E-01	25	L009	1 0 0 1 1	

4456. $C_{26}H_{38}O_4$
Trimethylcyclohexyl phthalate
bis(*cis*-3,3,5-Trimethylcyclohexyl) phthalate
RN: 245652-81-7 **MP** (°C)**:** 93
MW: 414.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-07	1.200E-04	24	H116	2 1 0 0 2	

4457. $C_{26}H_{38}O_6$
Hydrocortisone valerate
Hydrocortisone-21-valerate
RN: 6678-00-8 **MP** (°C)**:**
MW: 446.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.830E-06	3.050E-03	25	H098	1 0 2 0 2	
6.830E-06	3.050E-03	25	H320	0 0 0 0 0	
6.780E-06	3.028E-03	25	H320	0 0 0 0 0	

4458. $C_{26}H_{39}NO_3S$
4-Pregnene-20-one-3-spiro-2′-(4′-ethoxycarbonyl-1′,3′-thiazolidine)
RN: **MP** (°C)**:** 131–135
MW: 445.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.81E-06	~1.70E-03	ns	B199	0 0 0 0 0	

4459. $C_{26}H_{43}NO_3$
Acetaminophen stearate
Acetaminophen octadecanoate
Stearoyl acetaminophen
Octadecanoic acid, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, stearate (ester)
RN: 20675-22-3 **MP** (°C)**:** 117
MW: 417.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-05	5.000E-03	25	B010	1 1 1 1 0	
3.592E-05	1.500E-02	37	D029	0 0 0 0 0	

4460. $C_{26}H_{43}NO_6$
Glycocholic acid
Glycine, *N*-[(3α,5β,7α,12α)-3,7,12-trihydroxy-24-oxocholan-24-yl]-
RN: 475-31-0 **MP** (°C)**:** 130
MW: 465.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.085E-04	3.299E-01	20	E035	1 2 0 0 1	
2.188E-03	1.019E+00	60	E035	1 2 0 0 2	
5.035E-03	2.344E+00	80	E035	1 2 0 0 2	
1.810E-02	8.428E+00	100	E035	1 2 0 0 1	

4461. $C_{26}H_{50}O_4$

Dioctyl sebacate
Sebacic acid bis(2-ethylhexyl) ester
RN: 122-62-3 **MP** (°C)**:** –67
MW: 426.69 **BP** (°C)**:** 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-07	1.000E-04	25	F067	1 0 2 2 0	

4462. $C_{26}H_{56}O_2P_2$

bis(Di-*n*-hexyl-phosphinyl)ethane
HDPE
RN: 2785-34-4 **MP** (°C)**:**
MW: 462.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.300E-02	0	O002	2 0 2 2 1	EFG
6.484E-06	3.000E-03	25	O002	2 0 2 2 1	
6.484E-06	3.000E-03	60	O002	2 0 2 2 1	EFG

4463. $C_{27}H_{22}Cl_2N_4$

Clofazimine
Lamprene
N,5-bis(4-Chlorophenyl)-3,4-dihydro-3-((1-methylethyl)imino)-2-phenazinamine
3-(*p*-Chloroanilino)-10-(*p*-chlorophenyl)-2,10-dihydro-2-(isopropylimino)phenazine
RN: 2030-63-9 **MP** (°C)**:** 211
MW: 473.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.11E-06	<1.00E-03	ns	B404	0 2 1 1 0	
2.112E-05	1.000E-02	ns	K444	0 0 0 0 0	
2.000E-04	9.468E-02	ns	O322	0 0 0 0 0	EFG

4464. $C_{27}H_{29}NO_{11}$

Adriamycin
Adriblastin
RN: 23214-92-8 **MP** (°C)**:** 205
MW: 543.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.607E-02	1.961E+01	ns	I312	0 0 0 0 0	

4465. $C_{27}H_{30}O_3$
Norethindrone benzoate
RN: **MP** (°C)**:**
MW: 402.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.019E-08	8.128E-06	25	L078	1 0 1 2 2	

4466. $C_{27}H_{32}N_4O_2$
Butyldiantipyrylmethane
BDAM
RN: 61358-30-3 **MP** (°C)**:**
MW: 444.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.748E-05	3.000E-02	20	P054	0 0 0 0 0	

4467. $C_{27}H_{32}N_4O_2$
Isobutyldiantipyrylmethane
IBDAM
RN: 16671-34-4 **MP** (°C)**:**
MW: 444.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	6.000E-02	20	P054	0 0 0 0 0	

4468. $C_{27}H_{32}N_4S_2$
Isobutyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-(3-methylbutylidene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 73429-89-7 **MP** (°C)**:** 209
MW: 476.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	7.627E-02	ns	D087	0 2 0 0 1	

4469. $C_{27}H_{32}O_{14}$
Naringin
4H-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (*S*)-
RN: 10236-47-2 **MP** (°C)**:**
MW: 580.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.700E-01	6	P070	1 2 1 1 1	
8.613E-04	5.000E-01	20	P070	1 2 1 1 1	
1.361E-03	7.900E-01	35	P070	1 2 1 1 1	
3.376E-03	1.960E+00	45	P070	1 2 1 1 2	
1.233E-02	7.160E+00	55	P070	1 2 1 1 2	
7.271E-02	4.221E+01	65	P070	1 2 1 1 2	
1.864E-01	1.082E+02	75	P070	1 2 1 1 2	

4470. $C_{27}H_{33}N_3O_8$
Rolitetracycline
N-(1-Pyrrolidinylmethyl)tetracycline
Syntetrin
Tetraverin
Synotodecin
RN: 751-97-3 **MP** (°C)**:** 162dec
MW: 527.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.79E-02	>2.00E+01	21	M044	2 0 2 2 0	

4471. $C_{27}H_{34}O_3$
Testosterone phenylacetate
Androst-4-en-3-one, 17-[(phenylacetyl)oxy]-, (17β)-
RN: 5704-03-0 **MP** (°C)**:**
MW: 406.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-05	8.970E-03	25	L342	1 0 1 1 2	
2.188E-05	8.895E-03	ns	R427	0 0 0 0 0	

4472. $C_{27}H_{34}O_{10}$
Cortisone tricarballylate
RN: **MP** (°C)**:**
MW: 518.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	7.000E-02	25	M023	1 0 2 1 0	

4473. $C_{27}H_{36}N_2O_4$
Repaglinide
RN: 135062-02-1 **MP** (°C)**:**
MW: 452.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.988E-04	8.999E-02	25	M448	0 0 0 0 0	Intrinsic, EFG

4474. $C_{27}H_{38}N_2O_6$
p-Ureidophenyl prostaglandin E2
RN: **MP** (°C)**:**
MW: 486.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	1.363E-02	25	A066	1 0 1 1 1	

4475. $C_{27}H_{38}O_3$
Norethindrone heptanoate
RN: **MP** (°C)**:**
MW: 410.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	6.026E-05	25	L078	1 0 1 2 2	

4476. $C_{27}H_{40}N_2O_6$
p-Ureidophenyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 488.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-05	3.372E-02	25	A066	1 0 1 1 1	

4477. $C_{27}H_{40}O_6$
Hydrocortisone tebutate
Hydrocortisone-21-hexanoate
Hydrocortisone-21-caproate
RN: 508-96-3 **MP** (°C)**:** 168
MW: 460.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.083E-06	1.420E-03	25	H098	1 0 2 0 2	
3.083E-06	1.420E-03	25	H320	0 0 0 0 0	
3.060E-06	1.409E-03	25	H320	0 0 0 0 0	

4478. $C_{27}H_{42}Cl_2N_2O_6$
α-Chloramphenicol palmitate
β-Chloramphenicol palmitate
Chloramphenicol palmitate
RN: 530-43-8 **MP** (°C)**:** 359
MW: 561.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	6.177E-06	20	M006	2 2 1 2 1	
8.500E-08	4.773E-05	20	M006	2 2 1 2 1	
1.500E-08	8.423E-06	25	M006	2 2 1 2 1	
9.600E-08	5.391E-05	25	M006	2 2 1 2 1	
7.123E-06	4.000E-03	28	R004	0 0 0 0 0	
1.800E-08	1.011E-05	29	M006	2 2 1 2 1	
1.440E-07	8.086E-05	29	M006	2 2 1 2 2	
2.700E-08	1.516E-05	32	M006	2 2 1 2 1	
2.600E-07	1.460E-04	32	M006	2 2 1 2 2	
3.100E-08	1.741E-05	35	M006	2 2 1 2 1	
3.800E-07	2.134E-04	35	M006	2 2 1 2 2	

4479. $C_{27}H_{42}N_4O_7.0.3H_2O$
2′-(2-Heptanoyl-2-hexanyl-acetyl)-6-methoxypurine arabinoside (0.3 hydrate)
RN: 145913-52-6 **MP** (°C)**:**
MW: 540.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-04	1.615E-01	37	C348	0 0 0 0 0	pH 7.00

4480. $C_{27}H_{42}O_3$
Diosgenin
(25*R*)-Spirost-5-en-3β-ol
RN: 512-04-9 **MP** (°C)**:** 204
MW: 414.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-08	2.000E-05	25	L033	1 0 2 1 0	

4481. $C_{27}H_{42}O_3$
Nandrolone nonanoate
RN: **MP** (°C)**:**
MW: 414.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-06	9.260E-04	37	C026	0 0 0 0 0	

4482. $C_{27}H_{43}NO_8$
N-Methylglucamine testosterone
17-β-(4-Androsten-3-one)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 183–185
MW: 509.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.633E-05	4.400E-02	25	L009	1 0 0 1 1	

4483. $C_{27}H_{44}N_4O_6$
2′-Hexadecyl-6-methoxypurine arabinoside
RN: 145913-43-5 **MP** (°C)**:** 97–99
MW: 520.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	9.893E-03	37	C348	0 0 0 0 0	pH 7.00

4484. $C_{27}H_{44}O$
Vitamin D3
Cholecalciferol
Activated 7-dehydrocholesterol
Oleovitamin D3
RN: 67-97-0 **MP** (°C)**:** 85
MW: 384.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.30E-01	25	P312	0 0 0 0 0	

4485. $C_{27}H_{58}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)propane
HDPP
RN: 2896-56-2 **MP** (°C)**:**
MW: 476.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-04	1.300E-01	0	O002	2 0 2 2 0	EFG
1.154E-04	5.500E-02	15	O002	2 0 2 2 0	EFG
3.566E-05	1.700E-02	25	O002	2 0 2 2 0	

4486. $C_{28}H_{29}F_2N_3O$
Pimozide
2-Benzimidazolinone, 1-[1-[4,4-bis(*p*-fluorophenyl)butyl]-4-piperidyl]-
Orap
RN: 2062-78-4 **MP** (°C)**:**
MW: 461.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.900E-03	30	P044	0 0 0 0 0	

4487. $C_{28}H_{31}FN_4O$
Astemizole
1-((4-Fluorophenyl)-methyl)-*N*-(1-(2-(4-methoxyphenyl)ethyl)-4-piperidinyl)-1H-benzimidazol-2-amine
Hismanal
RN: 68844-77-9 **MP** (°C)**:**
MW: 458.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	3.210E-01	30	A417	0 0 0 0 0	pH 5.8
3.700E-03	1.697E+00	30	A417	0 0 0 0 0	pH 3.8

4488. $C_{28}H_{36}O_3$
Testosterone phenyl propionate
Androst-4-en-3-one, 17-(1-oxo-3-phenylpropoxy)-, (17β)-
RN: 1255-49-8 **MP** (°C)**:**
MW: 420.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.350E-06	2.250E-03	25	L342	1 0 1 1 2	

4489. $C_{28}H_{36}O_{15}$
Neohesperidin dihydrochalcone
1-Propanone, 1-[4-[[2-*O*-(6-deoxy-a-L-mannopyranosyl)-b-D-glucopyranosyl]oxy]-2,6-dihydroxyphenyl]-3-(3-hydroxy-4-methoxyphenyl)-
Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-(6-deoxy-a-L-mannopyranosyl)-, b-D-
Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-a-L-rhamnopyranosyl-
Neohesperidin DHC
NHDC
RN: 20702-77-6 **MP** (°C)**:**
MW: 612.59 **BP** (°C)**:** 927.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.530E-06	4.000E-03	rt	B417	0 0 1 2 1	

4490. $C_{28}H_{38}N_6O_{11}S$

Sildenafil citrate

1-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo [4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl] sulfonyl]-4-methylpiperazine citrate

Viagra

RN: 171599-83-0 **MP** (°C)**:**

MW: 666.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.231E-03	3.488E+00	ns	S469	0 0 0 0 0	

4491. $C_{28}H_{39}NO_6$

p-Acetamidophenyl prostaglandin E2

RN: **MP** (°C)**:**

MW: 485.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	2.622E-02	25	A066	1 0 1 1 1	

4492. $C_{28}H_{39}NO_6$

2-Oxo-5-indolinyl prostaglandin F2α

Prosta-5,13-dien-1-oic acid, 9,11,15-trihydroxy-, 2,3-dihydro-2-oxo-1H-indol-5-yl ester, (5Z,9α,11α,13E,15S)-

RN: 74973-22-1 **MP** (°C)**:**

MW: 485.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	2.914E-02	25	A066	1 0 1 1 1	

4493. $C_{28}H_{39}N_3O_6$

α-Semicarbazono-*p*-tolyl prostaglandin E2

RN: **MP** (°C)**:**

MW: 513.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	1.284E-03	25	A066	1 0 1 1 1	

4494. $C_{28}H_{40}FNO_{11}.H_2O$

Glucosamine 9-α-fluorohyfrocortisome (monohydrate)

21-(9-α-Fluoro-11α, 17α-dihydroxy-4-pregnen-3,20-dione)-*N*-2-(2-desoxyglucosyl) carbamate

RN: **MP** (°C)**:** 176-178

MW: 603.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.964E-04	3.600E-01	25	L009	1 0 0 1 1	

4495. $C_{28}H_{41}N_3O_6$
α-Semicarbazono-*p*-tolyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 515.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	8.250E-03	25	A066	1 0 1 1 1	

4496. $C_{28}H_{42}FNO_{11}.H_2O$
Glucamine 9-α-fluorohyfrocortisome (monohydrate)
RN: **MP** (°C)**:** 105–110
MW: 605.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.456E-03	2.699E+00	25	L009	1 0 0 1 1	

4497. $C_{28}H_{42}O_6$
Hydrocortisone heptanoate
Hydrocortisone-21-heptanoate
RN: **MP** (°C)**:**
MW: 474.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.082E-06	9.880E-04	25	H098	1 0 2 0 2	
2.082E-06	9.880E-04	25	H320	0 0 0 0 0	
2.060E-06	9.778E-04	25	H320	0 0 0 0 0	

4498. $C_{28}H_{44}O_3$
Nandrolone decanoate
Deca-durabolin
Norandrostenolone decanoate
RN: 360-70-3 **MP** (°C)**:**
MW: 428.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-06	6.640E-04	37	C026	0 0 0 0 0	

4499. $C_{28}H_{46}O_4$
Di-*n*-decyl phthalate
RN: 84-77-5 **MP** (°C)**:**
MW: 446.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.388E-07	3.300E-04	24	H116	2 1 0 0 2	

4500. $C_{28}H_{46}O_4$
Diisodecyl phthalate
RN: 26761-40-0 **MP** (°C)**:**
MW: 446.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.269E-07	2.800E-04	24	H116	2 1 0 0 2	

4501. $C_{28}H_{60}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)butane
HDPB
RN: 2785-35-5 **MP** (°C)**:**
MW: 490.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-04	1.780E-01	0	O002	2 0 2 2 0	EFG
1.284E-04	6.300E-02	15	O002	2 0 2 2 0	EFG
4.076E-05	2.000E-02	25	O002	2 0 2 2 0	

4502. $C_{29}H_{20}N_2O_4$
1,4-Dibenzoylaminoanthraquinone
Benzamide, *N*,*N*′-(9,10-dihydro-3-methyl-9,10-dioxo-1,8-anthracenediyl)bis
RN: 4627-15-0 **MP** (°C)**:**
MW: 460.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	1.013E-02	50	G077	1 0 0 0 1	

4503. $C_{29}H_{27}N_5O_4$
m-Nitrophenyldiantipyrylmethane
m-NPhDAM
RN: 1606-53-7 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.887E-05	3.000E-02	20	P054	0 0 0 0 0	

4504. $C_{29}H_{27}N_5O_4$
o-Nitrophenyldiantipyrylmethane
o-NPhDAM
RN: 14957-18-7 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4505. $C_{29}H_{27}N_5O_4$
p-Nitrophenyldiantipyrylmethane
p-NPhDAM
RN: 55774-19-1 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4506. $C_{29}H_{28}N_4O_2$
Phenyldiantipyrylmethane
PhDAM
RN: 1861-84-3 **MP** (°C)**:**
MW: 464.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.165E-04	2.399E-01	20	P054	0 0 0 0 0	

4507. $C_{29}H_{28}N_4O_3$
o-Hydroxylphenyldiantipyrylmethane
o-HPhDAM
RN: 1606-55-9 **MP** (°C)**:**
MW: 480.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.08E-05	<1.00E-02	20	P054	0 0 0 0 0	

4508. $C_{29}H_{28}N_4S_2$
Phenyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-(phenylmethylene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-68-1 **MP** (°C)**:** 160
MW: 496.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-05	2.086E-02	ns	D087	0 2 0 0 1	

4509. $C_{29}H_{32}O_{13}$
Etoposide
4′-Demethylepipodophyllotoxin ethylidene-β-D-glucoside
Vepesid
VP-16
RN: 33419-42-0 **MP** (°C)**:** 236–251
MW: 588.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-04	1.145E-01	25	S466	0 0 0 0 0	
3.398E-04	2.000E-01	ns	D347	0 0 0 0 0	
3.388E-04	1.994E-01	ns	R427	0 0 0 0 0	

4510. $C_{29}H_{35}NO_2$
Mifepristone
RU-486
RN: 84371-65-3 **MP** (°C)**:**
MW: 429.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.748E-04	22.5	B440	0 0 0 0 0	

4511. $C_{29}H_{36}N_4O_2$
Hexyldiantipyrylmethane
HDAM
RN: 7660-44-8 **MP** (°C)**:**
MW: 472.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.230E-05	1.999E-02	20	P054	0 0 0 0 0	
4.232E-05	2.000E-02	20	P054	0 0 0 0 0	

4512. $C_{29}H_{36}N_4S_2$
Hexyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-heptylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-69-2 **MP** (°C)**:** 169
MW: 504.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	2.070E-02	0	D087	0 2 0 0 1	

4513. $C_{29}H_{38}Cl_2N_2O_3$

3β-Hydroxy-13α-amino-13,17-seco-5α-androstan-17-oic-13,17-lactam-4-*N*,*N*-*bis*-(chloroethyl) amino phenyl-acetate

RN: **MP** (°C)**:**
MW: 533.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.186E-07	1.700E-04	25	P022	0 0 0 0 0	
3.599E-07	1.920E-04	30	P022	0 0 0 0 0	
4.517E-07	2.410E-04	44	P022	0 0 0 0 0	
6.110E-07	3.260E-04	73	P022	0 0 0 0 0	

4514. $C_{29}H_{38}O_3$

Testosterone phenylbutyrate

RN: **MP** (°C)**:**
MW: 434.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.681E-06	1.600E-03	25	L342	1 0 1 1 2	

4515. $C_{29}H_{40}N_2O_4$

Emetine
Emetan, 6′,7′,10,11-tetramethoxy-
NSC 33669

RN: 483-18-1 **MP** (°C)**:** 74
MW: 480.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	9.613E-01	15	K059	2 2 2 0 0	
2.078E-03	9.990E-01	c	D004	0 0 0 0 0	

4516. $C_{29}H_{42}O_6$

Cortisone caprylate

RN: **MP** (°C)**:**
MW: 486.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.110E-06	2.000E-03	25	M023	1 0 2 1 0	

4517. $C_{29}H_{44}FNO_{11}.H_2O$
N-Methylglucamine 9-α-fluorohyfrocortisome (monohydrate)
21-(9-α-Fluoro-11β, 17α-dihydroxy-4-pregnen-3,20-dione)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 120
MW: 619.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.358E-03	3.940E+00	25	L009	1 0 0 1 1	

4518. $C_{29}H_{44}O_{12}$
Oubain
γ-Strophanthin
Ouabain
Quabain
RN: 630-60-4 **MP** (°C)**:** 185
MW: 584.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.223E-02	1.300E+01	25	P312	0 0 0 0 0	
1.693E-02	9.901E+00	c	D004	0 0 0 0 0	
2.851E-01	1.667E+02	h	D004	0 0 0 0 0	

4519. $C_{29}H_{46}N_4O_7.0.4H_2O$
2′-(2-Octanoyl-2-heptanyl-acetyl)-6-methoxypurine arabinoside (0.4 hydrate)
RN: 145913-53-7 **MP** (°C)**:**
MW: 569.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.601E-02	37	C348	0 0 0 0 0	pH 7.00

4520. $C_{29}H_{46}O_3$
Nandrolone undecanoate
RN: **MP** (°C)**:**
MW: 442.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-06	6.020E-04	37	C026	0 0 0 0 0	

4521. $C_{29}H_{50}O_2$
Vitamin E
α-Tocopherol
RN: 59-02-9 **MP** (°C)**:**
MW: 430.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.833E-05	2.082E-02	33	D404	2 1 2 2 2	
4.852E-05	2.090E-02	33	D404	2 1 2 2 2	

4522. $C_{30}H_{28}N_4O_3$
Benzoyldiantipyrylmethane
BenzDAM
RN: 55774-17-9 **MP** (°C)**:**
MW: 492.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.03E-05	<1.00E-02	20	P054	0 0 0 0 0	

4523. $C_{30}H_{30}N_{20}O_{10}$
Cucurbit[5]uril
RN: 259886-49-2 **MP** (°C)**:**
MW: 830.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	3.406E-01	25	B424	1 0 1 2 2	

4524. $C_{30}H_{34}O_{13}$
Picrotoxin
Picrotoxine
RN: 124-87-8 **MP** (°C)**:**
MW: 602.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.964E-03	2.991E+00	20	D041	1 0 0 0 0	
6.776E-03	4.083E+00	rt	D021	0 0 1 1 1	

4525. $C_{30}H_{48}O_3$
β-Boswellic acid
RN: **MP** (°C)**:**
MW: 456.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	7.764E+00	ns	R422	0 0 0 0 0	

4526. $C_{30}H_{48}O_{12}$
Periplocin
Card-20(22)-enolide, 3-[(2,6-dideoxy-4-*O*-β-D-glucopyranosyl-3-*O*-methyl-β-D-ribo-hexopyranosyl)oxy]-5,14-dihydroxy-, (3β,5β)-
Periplocoside
RN: 13137-64-9 **MP** (°C)**:** 205
MW: 600.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.321E-02	7.937E+00	c	D004	0 0 0 0 0	

4527. $C_{31}H_{33}N_5O_2$
p-Dimethylaminophenyldiantipyrylmethane
p-DMAPhDAM
RN: 2088-76-8 **MP** (°C)**:**
MW: 507.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.576E-04	7.999E-02	20	P054	0 0 0 0 0	

4528. $C_{31}H_{38}N_2O_{11}$
Dihydronovobiocin
Benzamide, *N*-[7-[[3-*O*-(aminocarbonyl)-6-deoxy-5-C-methyl-4-*O*-methyl-β-L-lyxo-hexopyranosyl]oxy]-4-hydroxy-8-methyl-2-oxo-2H-1-benzopyran-3-yl]-4-hydroxy-3-(3-methylbutyl)-
RN: 29826-16-2 **MP** (°C)**:**
MW: 614.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.800E-01	28	A038	2 0 1 1 2	

4529. $C_{31}H_{42}FNO_{12}.H_2O$
Glucosamine triamcinolone acetonide (monohydrate)
21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-2-(2-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 250–255
MW: 657.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.717E-04	3.760E-01	25	L009	1 0 0 1 1	

4530. $C_{31}H_{44}FNO_{12}.H_2O$
Glucaminetriamcinolone acetonide (monohydrate)
21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 150
MW: 659.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.366E-03	3.540E+00	25	L009	1 0 0 1 1	

4531. $C_{31}H_{44}N_2O_7$
N-Acetyl-L-tyrosinamide prostaglandin E2
RN: **MP** (°C)**:**
MW: 556.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	9.464E-02	25	A066	1 0 1 1 1	

4532. $C_{31}H_{46}N_2O_7$
N-Acetyl-L-tyrosinamide prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 558.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	7.822E-02	25	A066	1 0 1 1 1	

4533. $C_{31}H_{48}O_{12}$
Strophanthin
k-Strophanthin
RN: 11005-63-3 **MP** (°C)**:** 179
MW: 612.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	2.273E+01	25	D004	0 0 0 0 0	

4534. $C_{32}H_{32}O_{14}$
Chartreusin
Lambdamycin
NSC 5159
Antibiotic X 465A
RN: 6377-18-0 **MP** (°C)**:** 246–249
MW: 640.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-05	1.500E-02	25	P067	0 0 0 0 0	

4535. $C_{32}H_{37}NO_5S$
Dextropropoxyphene napsylate
Darvocet N-50
Darvocet N-100
Darvon-N
RN: 17140-78-2 **MP** (°C)**:**
MW: 547.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-03	1.400E+00	22	N319	0 0 0 0 0	

4536. $C_{32}H_{40}BrN_5O_5$
Bromocriptine
2-Bromo-α-ergocryptine
Parlodel
Kripton
(5′α)-2-Bromo-12′-hydroxy-2′-(1-methylethyl)-5′-(2-methylpropyl)ergotaman-3′,6′,18-trione
RN: 25614-03-3 **MP** (°C)**:**
MW: 654.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-06	2.070E-03	ns	R427	0 0 0 0 0	

4537. $C_{32}H_{41}NO_2$
Terfenadine
Seldane
Teldane
RN: 50679-08-8 **MP** (°C)**:**
MW: 471.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-10	9.700E-08	25	A412	1 0 2 2 1	
		amb	L434	0 0 0 0 0	
2.138E-07	1.008E-04	ns	R427	0 0 0 0 0	

4538. $C_{32}H_{45}N_3O_4S$
Nelfinavir mesylate
Nelfinavir
NFV
Viracept
RN: 159989-65-8 **MP** (°C)**:**
MW: 567.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.925E-03	4.500E+00	ns	W424	0 0 0 0 0	

4539. $C_{32}H_{45}N_3O_4S$

Nelfinavir

(3*S*,4a*S*,8a*S*)-*N*-(1,1-Dimethylethyl)decahydro-2-[(2*R*,3*R*)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-(phenylthio)butyl]-3-isoquinolinecarboxamide

RN: 159989-64-7 **MP** (°C)**:**
MW: 567.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-02	7.000E+00	ns	A426	0 0 0 0 0	Intrinsic

4540. $C_{32}H_{46}FNO_{12}.H_2O$

N-Methylglucamine triamcinolone acetonide (monohydrate)

21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate

RN: **MP** (°C)**:** 152
MW: 673.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.744E-03	3.196E+00	25	L009	1 0 0 1 1	

4541. $C_{32}H_{49}NO_9$

Cevadine

Cevane-3,4,12,14,16,17,20-heptol, 4,9-epoxy-, 3-[(2Z)-2-methyl-2-butenoate], (3β,4α,16β)-

Veratrine

RN: 62-59-9 **MP** (°C)**:** 213.5
MW: 591.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	4.734E+00	15	K059	2 2 2 0 0	

4542. $C_{32}H_{54}O_4$

Didodecyl phthalate

1,2-Benzenedicarboxylic acid, didodecyl ester

RN: 2432-90-8 **MP** (°C)**:**
MW: 502.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-07	1.400E-04	24	H116	2 1 0 0 2	

4543. $C_{33}H_{25}N_3O_3$
Norbormide
5-(α-Hydroxy-α-2-pyridylbenzyl)-7-(α-2-pyridylbenzylidene)-5-norbornene-2,3-dicaboximide
Shoxin
RN: 991-42-4 **MP** (°C)**:** >160
MW: 511.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-04	6.000E-02	rt	M161	0 0 0 0 1	

4544. $C_{33}H_{34}O_3$
Norethindrone biphenyl-4-carboxylate
RN: **MP** (°C)**:**
MW: 478.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-09	3.715E-06	25	L078	1 0 1 2 2	

4545. $C_{33}H_{34}O_4$
Norethindrone 4-phenoxybenzoate
RN: **MP** (°C)**:**
MW: 494.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-07	7.079E-05	25	L078	1 0 1 2 2	

4546. $C_{33}H_{36}N_4O_6$
Bilirubin
21H-Biline-8,12-dipropanoic acid, 2,17-diethenyl-1,10,19,22,23,24-hexahydro-3,7,13,18-tetramethyl-1,19-dioxo-
RN: 635-65-4 **MP** (°C)**:**
MW: 584.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	4.093E-06	18	K104	1 0 0 0 2	intrinsic

4547. $C_{33}H_{40}N_2O_9$
Reserpine
3,4,5-Trimethoxybenzoyl methyl reserpate
Rauwilid
Rauwiloid
RN: 50-55-5 **MP** (°C)**:**
MW: 608.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	7.304E-02	30	L068	1 0 0 1 0	EFG
1.643E-05	1.000E-02	ns	K444	0 0 0 0 0	

4548. $C_{33}H_{41}N_5O_6S_2$
Kynostatin
KNI-272
4-Thiazolidinecarboxamide, *N*-(1,1-dimethylethyl)-3-[(2*S*,3*S*)-2-hydroxy-3-[[(2*R*)-2-[[(5-isoquinolinyloxy)acetyl]amino]-3-(methylthio)-1-oxopropyl]amino]-1-oxo-4-phenylbutyl]-, (4*R*)-
RN: 147318-81-8 **MP** (°C)**:**
MW: 667.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-06	4.200E-03	25	J308	0 0 0 0 0	

4549. $C_{33}H_{45}NO_9$
Delphinine
Indaconitine, *N*-deethyl-3-deoxy-*N*-methyl-
RN: 561-07-9 **MP** (°C)**:** 198–200
MW: 599.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.335E-05	2.000E-02	25	D004	0 0 0 0 0	

4550. $C_{33}H_{47}NO_{13}$
Natamycin
Pimafucin
RN: 7681-93-8 **MP** (°C)**:**
MW: 665.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-05	3.000E-02	20	B190	1 2 1 1 0	
6.159E-04	4.100E-01	21	M044	2 0 2 2 2	*sic*

4551. $C_{34}H_{30}N_2O_6S$

Pyrantel pamoate
Pirantel pamoate
Dog Wormer
Helmex
Lombriareu
Trilombrin

RN: 22204-24-6 **MP** (°C)**:** 266–267
MW: 594.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E-05	1.000E-02	ns	K444	0 0 0 0 0	

4552. $C_{34}H_{34}N_4O_4$

Protoprophyrin IX
Protoporphyrin IX

RN: 553-12-8 **MP** (°C)**:**
MW: 562.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	1.069E-01	25	C097	2 0 1 1 1	EFG

4553. $C_{34}H_{47}NO_{11}$

Aconitine
Acetylbenzoylaconine

RN: 302-27-2 **MP** (°C)**:** 204
MW: 645.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.691E-04	3.029E-01	25	D004	0 0 0 0 0	

4554. $C_{34}H_{50}O_7$

Carbenoxolone
Olean-12-en-29-oic acid, 3-(3-carboxy-1-oxopropoxy)-11-oxo-, (3β,20β)-

RN: 5697-56-3 **MP** (°C)**:**
MW: 570.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-05	6.621E-03	24	B363	0 0 0 0 0	
1.630E-05	9.304E-03	37	B363	0 0 0 0 0	

4555. $C_{34}H_{57}NO_7$
Glucosamine cholesterol
3-β-(5-Cholestenyl)-*N*-2-(2-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 155–158
MW: 591.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.530E-04	5.640E-01	25	L009	1 0 0 1 1	

4556. $C_{34}H_{58}O_4$
Ditridecyl phthalate
Staflex DTDP
Truflex DTDP
Hexaplas DTDP
Jayflex DTDP
Polycizer 962BPA
RN: 119-06-2 **MP** (°C)**:**
MW: 530.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.405E-07	3.400E-04	24	H116	2 1 0 0 2	

4557. $C_{34}H_{68}N_3O_8S_2$
Lincomycin hexadecylsulfamate
RN: **MP** (°C)**:**
MW: 711.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.738E-04	4.080E-01	21	M044	2 0 2 2 2	

4558. $C_{35}H_{44}N_2O_7$
p-(*p*-Acetamidobenzamido)phenyl prostaglandin E2
RN: **MP** (°C)**:**
MW: 604.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-08	5.927E-05	25	A066	1 0 1 1 1	

4559. $C_{35}H_{46}N_2O_7$
p-(*p*-Acetamidobenzamido)phenyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 606.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-07	1.699E-04	25	A066	1 0 1 1 1	

4560. $C_{35}H_{47}NO_9$
Rhizoxin
RN: 90996-54-6 **MP** (°C)**:**
MW: 625.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-05	1.200E-02	25	P336	0 0 0 0 0	

4561. $C_{35}H_{61}NO_7$
N-Methylglucamine cholesterol
3-β-(5-Cholestenyl)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 131–133
MW: 607.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-04	1.120E-01	25	L009	1 0 0 1 1	

4562. $C_{36}H_{47}N_2O_7$
N-Benzoyl-L-tyrosinamide prostaglandin E2
RN: **MP** (°C)**:**
MW: 619.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-07	2.913E-04	25	A066	1 0 1 1 1	

4563. $C_{36}H_{47}N_5O_4$
Indinavir sulfate
Crixivan
IDV
Indinavir
Indinavir sulfate
MK-639
RN: 157810-81-6 **MP** (°C)**:**
MW: 613.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.63E-01	>1.00E+02	ns	W424	0 0 0 0 0	

4564. $C_{36}H_{47}N_5O_4$
Indinavir
2,3,5-Trideoxy-*N*-[(1*S*,2*R*)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]-5-[(2*S*)-2-[[(1,1-dimethylethyl) amino]carbonyl]-4-(3-pyridinylmethyl)-1-piperazinyl]-2-(phenylmethyl)-D-erythro-pentonamide
N-(2-hydroxy-1(*S*)-indanyl)-2-(phenylmethyl)-4(*S*)-hydroxy-5-[1-[4-(3-pyridylmethyl)-2(*S*)-(*N*-*tert*-butylcarbamoyl)piperazinyl]]pentanamide
RN: 150378-17-9 **MP** (°C)**:**
MW: 613.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	7.000E-02	ns	A426	0 0 0 0 0	Intrinsic

4565. $C_{36}H_{49}N_2O_7$
N-Benzoyl-L-tyrosinamide prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 621.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	1.119E-03	25	A066	1 0 1 1 1	

4566. $C_{36}H_{56}O_{14}$
Digitalin
Card-20(22)-enolide, 3-[(6-deoxy-4-*O*-β-D-glucopyranosyl-3-*O*-methyl-β-D-galactopyranosyl) oxy]-14,16-dihydroxy-, (3β,5β,16β)-
Digitalinum verum
RN: 752-61-4 **MP** (°C)**:** 229
MW: 712.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.401E-03	9.990E-01	25	D004	0 0 0 0 0	

4567. $C_{36}H_{57}N_7O_{10}S$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(2-sulfoethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-, [1*S*-[1*R**,2*R**,4(*R**)]]-

RN: 100902-06-5 **MP** (°C)**:**
MW: 779.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.10E-02	>8.58E+00	ns	B425	0 0 0 1 0	

4568. $C_{36}H_{58}N_8O_7$

L-Leucinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3*S*,4*S*)-4-amino-3-hydroxy-6-methylheptanoyl-*N*-(2-aminoethyl)-

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[(2-aminoethyl)amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 105192-87-8 **MP** (°C)**:**
MW: 714.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	3.503E+00	ns	B425	0 0 0 1 0	pH 7.4

4569. $C_{36}H_{60}O_2$

Vitamin A palmitate
Retinol, hexadecanoate
Retinyl palmitate

RN: 79-81-2 **MP** (°C)**:**
MW: 524.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.624E-04	25	P343	0 0 0 0 0	
1.905E-05	1.000E-02	ns	K444	0 0 0 0 0	

4570. $C_{36}H_{60}O_{30}$

α-Cyclodextrin
β-Hexaamylose
(C6H10O5)6
α-Dextrin

RN: 10016-20-3 **MP** (°C)**:**
MW: 972.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.345E-02	9.091E+01	20	F186	1 2 1 1 1	
2.409E-02	2.344E+01	20	P048	1 0 1 1 1	*sic*
1.118E-01	1.088E+02	23.7	J305	0 0 0 0 0	
1.204E-01	1.171E+02	23.7	J305	0 0 0 0 0	
1.460E-01	1.420E+02	25	B396	0 0 0 0 0	

(*continued*)

4570. $C_{36}H_{60}O_{30}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-01	1.450E+02	25	L432	0 0 0 0 0	
1.800E-01	1.751E+02	25	O321	0 0 0 0 0	
1.331E-01	1.295E+02	25	S462	0 0 0 0 0	
1.211E-01	1.178E+02	25.0	J305	0 0 0 0 0	
1.318E-01	1.282E+02	25.0	J305	0 0 0 0 0	
1.678E-01	1.632E+02	30.0	J305	0 0 0 0 0	
1.501E-01	1.460E+02	30.0	J305	0 0 0 0 0	
1.696E-01	1.650E+02	33.0	J305	0 0 0 0 0	
1.912E-01	1.860E+02	33.0	J305	0 0 0 0 0	
2.161E-01	2.102E+02	35.0	J305	0 0 0 0 0	
1.885E-01	1.834E+02	35.0	J305	0 0 0 0 0	
2.331E-01	2.268E+02	38.0	J305	0 0 0 0 0	
2.023E-01	1.968E+02	38.0	J305	0 0 0 0 0	
2.100E-01	2.043E+02	40	O321	0 0 0 0 0	
2.171E-01	2.112E+02	40.0	J305	0 0 0 0 0	
2.532E-01	2.463E+02	40.0	J305	0 0 0 0 0	
2.229E-01	2.169E+02	42.0	J305	0 0 0 0 0	
2.616E-01	2.545E+02	42.0	J305	0 0 0 0 0	
2.677E-01	2.604E+02	43.0	J305	0 0 0 0 0	
2.283E-01	2.221E+02	43.0	J305	0 0 0 0 0	
2.492E-01	2.424E+02	45.0	J305	0 0 0 0 0	
2.982E-01	2.901E+02	45.0	J305	0 0 0 0 0	
3.397E-01	3.305E+02	48.0	J305	0 0 0 0 0	
2.773E-01	2.698E+02	48.0	J305	0 0 0 0 0	
4.700E-01	4.572E+02	55	O321	0 0 0 0 0	
1.302E-01	1.266E+02	ns	M335	0 0 2 0 1	
1.490E-01	1.450E+02	rt	F041	0 2 2 0 2	

4571. $C_{36}H_{72}N_3O_8S_2$

Lincomycin octadecylsulfamate

RN: **MP** (°C)**:**

MW: 739.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.897E-04	2.880E-01	21	M044	2 0 2 2 2	

4572. $C_{36}H_{74}$

n-Hexatriacontane

Hexatriacontane

RN: 630-06-8 **MP** (°C)**:** 75.0

MW: 506.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-09	1.700E-06	25	B069	1 0 1 1 1	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 2	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 0	

4573. $C_{37}H_{48}N_6O_5S_2$
Ritonavir
ABT-538
Norvir
Ritonavir
RN: 155213-67-5 **MP** (°C)**:**
MW: 720.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.935E-06	5.000E-03	ns	A426	0 0 0 0 0	intrinsic
1.387E-05	1.000E-02	ns	K444	0 0 0 0 0	
~1.39E+00	~9.99E+02	ns	W424	0 0 0 0 0	

4574. $C_{37}H_{67}NO_{13}.2H_2O$
Erythromycin (dihydrate)
RN: 114-07-8 **MP** (°C)**:**
MW: 769.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.857E-04	5.280E-01	30	F310	1 0 2 2 2	
4.922E-04	3.790E-01	40	F310	1 0 2 2 2	
4.377E-04	3.370E-01	50	F310	1 0 2 2 2	
4.143E-04	3.190E-01	60	F310	1 0 2 2 2	
4.598E-04	3.540E-01	70	F310	1 0 2 2 2	
5.688E-04	4.380E-01	80	F310	1 0 2 2 2	

4575. $C_{38}H_{50}N_6O_5$
Squinavir
Butanediamide, *N*1-[(1*S*,2*R*)-3-[(3*S*,4a*S*,8a*S*)-3-[[(1,1-dimethylethyl)amino]carbonyl]octahydro-2-(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-
Saquinavir mesylate
Fortovase
Invirase
(*S*)-*N*-[(a*S*)-a-[(1*R*)-2-[(3*S*,4a*S*,8a*S*)-3-(*tert*-Butylcarbamoyl)octahydro-2(1H)-isoquinolyl]-1-hydroxyethyl]phenethyl]-2-quinaldamidosuccinamide
RN: 127779-20-8 **MP** (°C)**:**
MW: 670.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.336E-05	3.580E-02	25	B431	1 0 1 1 0	
8.198E-05	5.500E-02	25	C437	0 0 0 0 0	Average
3.309E-03	2.220E+00	ns	W424	0 0 0 0 0	

4576. $C_{38}H_{60}N_8O_9$

Butanoic acid, *N*4-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-2,4-diamino-

RN: 115511-05-2 **MP** (°C)**:**
MW: 772.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	1.778E+00	ns	B425	0 0 0 1 0	pH 7.4

4577. $C_{38}H_{69}NO_{13}$

Clarithromycin
Biaxin
A-56268
TE-031

RN: 81103-11-9 **MP** (°C)**:** 218.5
MW: 747.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-04	9.948E-02	20	N334	0 0 0 0 0	EFG
1.089E-04	8.145E-02	37	N334	0 0 0 0 0	EFG
4.893E-05	3.660E-02	50	N334	0 0 0 0 0	EFG

4578. $C_{40}H_{51}NO_{14}$

Streptovaricin C
Streptovaricin

RN: 1404-74-6 **MP** (°C)**:** 189
MW: 769.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.604E-03	1.235E+00	21	M044	2 0 2 2 2	

4579. $C_{40}H_{58}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(2-pyridinylmethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-49-4 **MP** (°C)**:**
MW: 762.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	1.373E-01	ns	B425	0 0 0 1 0	pH 7.4

4580. $C_{40}H_{58}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(4-pyridinylmethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-50-7 **MP** (°C)**:**
MW: 762.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	2.594E-01	ns	B425	0 0 0 1 0	pH 7.4

4581. $C_{40}H_{58}N_8O_8$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[[(1-oxido-4-pyridinyl)methyl]amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100902-03-2 **MP** (°C)**:**
MW: 778.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	3.272E+00	ns	B425	0 0 0 1 0	pH 7.4

4582. $C_{41}H_{59}N_7O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[(phenylmethyl)amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 109585-11-7 **MP** (°C)**:**
MW: 761.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<7.62E-03	ns	B425	0 0 0 1 0	pH 7.4

4583. $C_{41}H_{61}N_9O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[2-amino-2-(2-pyridinyl)ethyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-99-3 **MP** (°C)**:**
MW: 792.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	3.168E-01	ns	B425	0 0 0 1 0	pH 7.4

4584. $C_{41}H_{64}O_{13}$

Digitoxin
(3β,5β)-3-[(0-2,6-Dideoxy-β-D-ribo-hexopyranosyl-(1->4)-*O*-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1->4)-2,6-dideoxy-β-D-ribo-hexopyranosyl)oxy]-14-hydroxycard-20(22)-enolide
Crystodigin
Digifortis
RN: 71-63-6 **MP** (°C)**:** 256
MW: 764.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.307E-05	1.000E-02	20	J010	1 0 0 0 0	
5.098E-06	3.900E-03	25	M301	1 1 2 2 1	anhydrate
2.000E-05	1.530E-02	30	O321	0 0 0 0 0	
2.222E-05	1.700E-02	30	O321	0 0 0 0 0	
1.447E-05	1.107E-02	37	C303	2 2 2 2 2	average of 3
3.255E-06	2.490E-03	37	M301	1 1 2 2 1	anhydrate
1.300E-05	9.944E-03	ns	M070	0 0 0 0 1	
9.151E-06	7.000E-03	ns	N302	0 2 1 2 0	

4585. $C_{41}H_{64}O_{14}$

Digoxin
3β-((*O*-2,6-Dideoxy-β-D-ribo-hexopyranosyl-(1->4)-*O*-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1->4)-2,6-dideoxy-β-D-ribo-hexopyranosyl)oxy)-12β,14-dihydroxy-5β-card-20(22)-enolide
Lanoxicaps
Lanoxin
RN: 20830-75-5 **MP** (°C)**:** 260
MW: 780.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	9.789E-02	25	F010	2 1 2 2 2	Swiss micron
6.786E-05	5.300E-02	25	F010	2 1 2 2 2	
7.375E-05	5.760E-02	25	F010	2 1 2 2 2	Swiss standard
8.297E-05	6.480E-02	25	F010	2 1 2 2 2	
1.000E-04	7.810E-02	25	H066	1 0 0 0 0	EFG
3.585E-05	2.800E-02	25	M301	1 1 2 2 1	
3.675E-05	2.870E-02	25	N301	2 0 2 2 2	
3.841E-05	3.000E-02	27	E052	2 0 2 2 0	EFG
3.585E-05	2.800E-02	30	O321	0 0 0 0 0	
4.000E-05	3.124E-02	30	O321	0 0 0 0 0	
6.312E-05	4.930E-02	37	C303	2 2 2 2 2	average of 6
3.457E-05	2.700E-02	37	M301	1 1 2 2 1	
3.483E-05	2.720E-02	37	N301	2 0 2 2 2	
4.443E-05	3.470E-02	37	R009	1 0 0 0 2	
2.817E-05	2.200E-02	100	D027	1 2 0 0 1	
1.268E-03	9.900E-01	amb	L434	0 0 0 0 0	
7.363E-06	5.750E-03	ns	F037	0 0 2 0 2	mp 225.5 C
8.963E-06	7.000E-03	ns	F037	0 0 2 0 2	mp 225.5 C
5.570E-06	4.350E-03	ns	F037	0 0 2 0 2	mp 228.5 C

(*continued*)

4585. $C_{41}H_{64}O_{14}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.915E-06	5.400E-03	ns	F037	0 0 2 0 2	mp 235.5 C
1.280E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.097E-05	3.200E-02	ns	N302	0 2 1 2 1	
5.900E-05	4.608E-02	rt	J034	0 0 0 0 0	

4586. $C_{41}H_{64}O_{14}$

Gitoxin
Anhydrogitalin
Pseudodigitoxin
Bigitalin

RN: 4562-36-1 **MP** (°C)**:**
MW: 780.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	2.343E-03	ns	M070	0 0 0 0 0	

4587. $C_{41}H_{67}NO_{15}$

Troleandomycin
Triacetyloleandomycin

RN: 2751-09-9 **MP** (°C)**:**
MW: 813.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.071E-04	2.500E-01	28	A038	2 0 1 1 1	

4588. $C_{41}H_{68}N_8O_9$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[3-[bis(2-hydroxyethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 87691-52-9 **MP** (°C)**:**
MW: 817.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	3.513E+00	ns	B425	0 0 0 1 0	

4589. $C_{42}H_{59}N_7O_9$

Glycine, *N*-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-D-2-phenyl-

RN: 115511-06-3 **MP** (°C)**:**
MW: 805.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-04	5.964E-01	ns	B425	0 0 0 1 0	

4590. $C_{42}H_{62}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-98-2 **MP** (°C)**:**
MW: 791.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	1.107E+00	ns	B425	0 0 0 1 0	pH 7.4

4591. $C_{42}H_{70}O_{35}$

β-Cyclodextrin
β-Cyclodextrin hydrate
Cycloheptaamylose hydrate
Cyclodextrin hydrate

RN: 7585-39-9 **MP** (°C)**:** 298–300
MW: 1135.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-02	1.185E+01	15	W317	2 2 1 0 2	
1.216E-02	1.381E+01	20	F186	1 2 1 1 1	
1.282E-02	1.455E+01	20	W317	2 2 1 0 2	
1.410E-02	1.600E+01	21	C407	1 0 1 2 1	
1.540E-02	1.748E+01	23.7	J305	0 0 0 0 0	
1.630E-02	1.850E+01	25	B396	0 0 0 0 0	
1.586E-02	1.800E+01	25	C407	1 0 1 2 1	
1.558E-02	1.768E+01	25	H319	0 0 0 0 0	
1.600E-02	1.816E+01	25	O304	1 2 2 2 2	
1.600E-02	1.816E+01	25	O321	0 0 0 0 0	
1.621E-02	1.840E+01	25	S462	0 0 0 0 0	
1.674E-02	1.900E+01	25	T425	0 0 0 0 0	
1.551E-02	1.760E+01	25	W317	2 2 1 0 2	
1.630E-02	1.850E+01	25.0	J305	0 0 0 0 0	
2.026E-02	2.300E+01	30	C407	1 0 1 2 1	
1.895E-02	2.151E+01	30	W317	2 2 1 0 2	
2.203E-02	2.500E+01	35	C407	1 0 1 2 1	
2.440E-02	2.769E+01	35.0	J305	0 0 0 0 0	
3.100E-02	3.519E+01	40	O321	0 0 0 0 0	
2.980E-02	3.382E+01	40.0	J305	0 0 0 0 0	

(*continued*)

4591. $C_{42}H_{70}O_{35}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.850E-02	4.370E+01	45.0	J305	0 0 0 0 0	
4.430E-02	5.028E+01	48.0	J305	0 0 0 0 0	
4.400E-02	4.994E+01	55	O321	0 0 0 0 0	
1.558E-02	1.768E+01	ns	M335	0 0 2 0 1	

4592. $C_{42}H_{70}O_{35}$

6-*O*-α-D-Glucosyl-α-cyclodextrin

RN: **MP** (°C)**:**

MW: 1135.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-01	9.080E+02	25	O321	0 0 0 0 0	
1.030E+00	1.169E+03	40	O321	0 0 0 0 0	
1.190E+00	1.351E+03	55	O321	0 0 0 0 0	

4593. $C_{43}H_{55}NO_{13}$

Docetaxel

Taxotere

N-Debenzoyl-*N*-*tert*-butoxycarbonyl-10-deacetyl taxol

RN: 114977-28-5 **MP** (°C)**:**

MW: 793.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.557E-06	6.000E-03	22.5	C438	0 0 0 0 0	

4594. $C_{43}H_{58}N_4O_{12}$

Rifampin

Rifampicin

RN: 13292-46-1 **MP** (°C)**:**

MW: 822.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-01	1.070E+02	25	B073	2 1 2 2 2	pH 2.12,*sic*
4.374E-03	3.600E+00	25	B073	2 1 2 2 1	pH 2.5
1.701E-03	1.400E+00	25	B073	2 1 2 2 1	pH 5.33
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.99
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.03
1.580E-03	1.300E+00	25	G096	1 0 0 0 0	pH 4.3
1.215E-04	1.000E-01	ns	K444	0 0 0 0 0	
3.393E-03	2.792E+00	rt	F182	0 0 0 0 1	pH 7.5

4595. $C_{43}H_{61}N_7O_{10}$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[[3-(carboxymethoxy) phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-, [1*S*-[1*R**,2*R**,4(*R**)]]-

RN: 100902-05-4 **MP** (°C)**:**
MW: 836.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	2.257E-01	ns	B425	0 0 0 1 0	

4596. $C_{43}H_{62}N_8O_7$

L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-*N*-[3-methyl-1-[[(4-pyridinylmethyl)amino]carbonyl]butyl]-

RN: 105192-86-7 **MP** (°C)**:**
MW: 803.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.03E-03	ns	B425	0 0 0 1 0	pH 7.4

4597. $C_{43}H_{62}N_8O_8$

L-Phenylalaninamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3*S*,4*S*)-4-amino-3-hydroxy-6-methylheptanoyl-L-leucyl-

L-Phenylalaninamide, *N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl] amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl-,

RN: **MP** (°C)**:**
MW: 819.02 **BP** (°C)**:** 1171.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-05	<1.64E-02	ns	B425	0 0 0 1 0	pH 7.4

4598. $C_{43}H_{75}NO_{16}$

Erythromycin ethyl succinate

RN: 1264-62-6 **MP** (°C)**:**
MW: 862.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	1.950E-01	21	M044	2 0 2 2 2	

4599. $C_{44}H_{56}O_4$

p-tert-Butylcalix[4]arenetetrol
Tetra-*p-tert*-butyltetracalix[4]arene
p-tert-Butylcalix[4]arene
p-tert-Butylcalix[4]arene-25,26,27,28-tetrol
Formaldehyde-*p-tert*-butylphenyl cyclic tetramer
5,11,17,23-Tetra-*p-tert*-butyl-25,26,27,28-tetrahydroxycalix(4)arene

RN: 60705-62-6 **MP** (°C)**:** 342–346
MW: 648.93 **BP** (°C)**:** 683.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<6.49E-03	25	B424	1 0 1 2 2	

4600. $C_{44}H_{64}N_8O_9$

D-Phenylalanine, 3-(aminomethyl)-*N*-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-

RN: 115511-03-0 **MP** (°C)**:**
MW: 849.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	3.311E-01	ns	B425	0 0 0 1 0	pH 7.4

4601. $C_{44}H_{69}NO_{10}$

Tacrolimus
FK506

RN: 104987-11-3 **MP** (°C)**:**
MW: 772.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-06	1.220E-03	25	A410	1 0 2 2 1	

4602. $C_{44}H_{74}O_{34}$

n-Ethyl-paba-β-cyclodextrin

RN: **MP** (°C)**:**
MW: 1147.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-03	5.850E+00	ns	F327	0 0 1 2 2	

4603. $C_{44}H_{74}O_{35}$
Hydroxyethyl-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1163.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-01	3.750E+02	ns	M335	0 0 2 0 1	

4604. $C_{45}H_{63}Cl_2NO_6$
Cosalane
RN: 154212-56-3 **MP** (°C)**:** 262 C
MW: 784.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.784E-09	1.400E-06	ns	V417	0 0 0 0 0	

4605. $C_{45}H_{66}N_8O_7$
L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[4-(phenylmethyl)-1-piperazinyl]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-
RN: 105192-85-6 **MP** (°C)**:**
MW: 831.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.31E-03	ns	B425	0 0 0 1 0	pH 7.4

4606. $C_{45}H_{66}N_8O_7$
L-threo-Pentonamide, *N*-[1-[[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]-5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-
RN: 100902-07-6 **MP** (°C)**:**
MW: 831.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	1.662E-02	ns	B425	0 0 0 1 0	pH 7.4

4607. $C_{45}H_{73}NO_{15}$
Solanine
β-D-Galactopyranoside, (3β)-solanid-5-en-3-yl *O*-6-deoxy-α-L-mannopyranosyl-(1®2)-*O*-[β-D-glucopyranosyl-(1-3)]-
Solanidane, β-D-galactopyranoside deriv
RN: 20562-02-1 **MP** (°C)**:**
MW: 868.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.604E-02	15	K059	2 2 2 0 0	

4608. $C_{45}H_{76}O_{35}$
n-Propyl-paba-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1177.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	2.472E+00	ns	F327	0 0 1 2 2	

4609. $C_{46}H_{62}N_4O_{11}$
Rifabutin
1′,4-Didehydro-1-deoxy-1,4-dihydro-5′-(2-methylpropyl)-1-oxo
Ansamycin
Antibiotic LM 427
LM 427
Mycobutin
RN: 72559-06-9 **MP** (°C)**:**
MW: 847.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E-04	1.900E-01	ns	S469	0 0 0 0 0	

4610. $C_{46}H_{65}N_7O_{10}$
Acetic acid, [3-[[[2-[[5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-L-threo-pentonoyl]amino]-4-methyl-1-oxopentyl]amino]methyl]phenoxy]-
RN: 100902-09-8 **MP** (°C)**:**
MW: 876.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.628E-02	ns	B425	0 0 0 1 0	

4611. $C_{46}H_{77}NO_{17}$
Tylosin
Vubityl 200
Vetil(R)
RN: 1401-69-0 **MP** (°C)**:** 128
MW: 916.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.195E-03	7.508E+00	21	M044	2 0 2 2 2	

4612. $C_{46}H_{78}O_{35}$
n-Butyl-paba-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1191.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	8.338E-01	ns	F327	0 0 1 2 2	

4613. $C_{47}H_{51}NO_{14}$
Paclitaxel
5-β,20-Epoxy-1,2-α,4,7-β,10-β,13-α-hexahydroxy-tax-11-en-9-one 4,10-diacetate 2-benzoate 13-ester with (2*R*,3*S*)-*N*-benzoyl-3-phenyl-isoserine
TAX
Taxal
Taxol
Taxol A
RN: 33069-62-4 **MP** (°C)**:** 213–216
MW: 853.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-07	3.000E-04	37	L435	0 0 0 0 0	
1.569E-06	1.340E-03	37	V412	0 0 0 0 0	

4614. $C_{47}H_{73}NO_{17}$
Amphotericin B
RN: 1397-89-3 **MP** (°C)**:**
MW: 924.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.116E-04	7.500E-01	28	A038	2 0 1 1 1	
3.246E-06	3.000E-03	ns	K067	0 0 2 1 0	intrinsic

4615. $C_{47}H_{75}NO_{17}$

Nystatin
Mycostatin
Biofanal
Nystex
Fungicidin

RN: 1400-61-9 **MP** (°C)**:**
MW: 926.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	3.600E-01	24	M166	2 0 0 0 1	
4.319E-03	4.000E+00	ns	K444	0 0 0 0 0	

4616. $C_{48}H_{72}O_{14}$

Ivermectin
Heartgard-30
Ivomec

RN: 70288-86-7 **MP** (°C)**:**
MW: 873.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-06	4.000E-03	ns	K444	0 0 0 0 0	

4617. $C_{48}H_{80}O_{40}$

6-*O*-α-D-Maltosyl-α-cyclodextrin
6-*O*-α-Maltosyl-α-cyclodextrin

RN: **MP** (°C)**:**
MW: 1297.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-01	9.988E+02	25	O321	0 0 0 0 0	
2.400E-01	3.113E+02	25	O321	0 0 0 0 0	
7.700E-01	9.988E+02	40	O321	0 0 0 0 0	
3.500E-01	4.540E+02	40	O321	0 0 0 0 0	
1.330E+00	1.725E+03	55	O321	0 0 0 0 0	
5.400E-01	7.005E+02	55	O321	0 0 0 0 0	

4618. $C_{48}H_{80}O_{40}$

γ-Cyclodextrin
Cyclooctaamylose
Ringdex C
Cyclomaltooctaose
Dexy Pearl γ-100

RN: 17465-86-0 **MP** (°C)**:**
MW: 1297.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.338E-01	1.736E+02	20	F186	1 2 1 1 1	
1.789E-01	2.320E+02	25	B396	0 0 0 0 0	
2.000E-01	2.594E+02	25	O321	0 0 0 0 0	
1.921E-01	2.492E+02	25	S462	0 0 0 0 0	
1.680E-01	2.179E+02	25.0	J305	0 0 0 0 0	
2.040E-01	2.646E+02	30.0	J305	0 0 0 0 0	
2.430E-01	3.152E+02	35.0	J305	0 0 0 0 0	
4.300E-01	5.578E+02	40	O321	0 0 0 0 0	
2.680E-01	3.476E+02	40.0	J305	0 0 0 0 0	
3.110E-01	4.034E+02	42.0	J305	0 0 0 0 0	
6.400E-01	8.302E+02	55	O321	0 0 0 0 0	
1.452E-01	1.883E+02	ns	M335	0 0 2 0 1	

4619. $C_{49}H_{87}NS$

Erythromycin lactobionate

RN: 3847-29-8 **MP** (°C)**:** 145
MW: 722.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.77E-02	>2.00E+01	21	M044	2 0 2 2 0	

4620. $C_{50}H_{82}N_{10}O_{31}S_{10}$

Decane(*S*-(carboxymethyl)-L-cysteine))

RN: **MP** (°C)**:**
MW: 1639.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E-05	9.544E-02	15	N331	0 0 0 0 0	
5.730E-04	9.397E-01	25	N331	0 0 0 0 0	

4621. $C_{51}H_{55}NO_{18}$
7-Malyl paclitaxel
RN: 265659-44-7 **MP** (°C)**:** 166–168
MW: 970.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.093E-04	3.000E-01	ns	D401	0 2 2 2 0	

4622. $C_{51}H_{55}NO_{18}$
2′-Malyl paclitaxel
RN: 265659-38-9 **MP** (°C)**:** 148–151
MW: 970.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-04	2.000E-01	ns	D401	0 2 2 2 0	

4623. $C_{51}H_{70}N_{12}O_{11}$
His-pro-D-phe-his-leu-leu-thr-tyr
RN: **MP** (°C)**:**
MW: 1027.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-05	8.320E-02	20	B141	1 2 0 0 1	pH 7.5

4624. $C_{51}H_{74}O_{19}$
Penta-acetyl-gitoxin
RN: 7242-04-8 **MP** (°C)**:**
MW: 991.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	1.189E-02	ns	M070	0 0 0 0 1	

4625. $C_{52}H_{72}N_{12}O_{10}$
His-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1025.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-04	1.651E-01	ns	B141	0 2 0 0 2	pH 7.5

4626. $C_{52}H_{72}N_{12}O_{10}$
His-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1025.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	1.405E-01	ns	B141	0 2 0 0 2	pH 7.5

4627. $C_{52}H_{88}O_{39}$
n-Butyl-paba-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1337.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	9.361E-01	ns	F327	0 0 1 2 2	

4628. $C_{52}H_{97}NO_{18}S$
Erythromycin estolate
RN: 3521-62-8 **MP** (°C)**:** 135
MW: 1056.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.515E-04	1.600E-01	21	M044	2 0 2 2 2	

4629. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Glucosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-01	1.430E+03	25	O321	0 0 0 0 0	
1.010E+00	1.474E+03	40	O321	0 0 0 0 0	
1.180E+00	1.722E+03	55	O321	0 0 0 0 0	

4630. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Maltosyl-β-cyclodextrin
6-*O*-α-Maltosyl-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.518E+03	25	O321	0 0 0 0 0	
1.040E+00	1.518E+03	40	O321	0 0 0 0 0	
1.220E+00	1.780E+03	55	O321	0 0 0 0 0	

4631. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Maltotriosyl-α-cyclodextrin
6-*O*-α-Maltotriosyl-α-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E+00	1.561E+03	25	O321	0 0 0 0 0	
1.220E+00	1.780E+03	40	O321	0 0 0 0 0	
1.370E+00	1.999E+03	55	O321	0 0 0 0 0	

4632. $C_{55}H_{59}NO_{22}$
2′,7-*bis*-(Malyl) paclitaxel
RN: 265659-41-4 **MP** (°C)**:** 166–168
MW: 1086.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.604E-04	5.000E-01	ns	D401	0 2 2 2 0	

4633. $C_{55}H_{70}N_{12}O_{10}$
His-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1059.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-04	1.864E-01	ns	B141	0 2 0 0 2	pH 7.5

4634. $C_{55}H_{79}N_{13}O_{11}$
His-pro-D-phe-his-leu-leu-val-tyr-serinol
RN: **MP** (°C)**:**
MW: 1098.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.295E-01	20	B141	1 2 0 0 2	pH 7.5

4635. $C_{55}H_{90}N_{11}O_{34}S_{11}$
Undecane(*S*-(carboxymethyl)-L-cysteine))
RN: **MP** (°C)**:**
MW: 1802.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-06	1.658E-02	15	N331	0 0 0 0 0	
1.340E-04	2.415E-01	25	N331	0 0 0 0 0	
2.900E-04	5.226E-01	35	N331	0 0 0 0 0	

4636. $C_{56}H_{98}O_{35}$
β-Cyclodextrin, tetradeca-*O*-methyl-
Heptakis(2,6-di-*O*-methyl)-β-cyclodextrin
RN: 188367-19-3 **MP** (°C)**:**
MW: 1331.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-01	3.631E+02	25	H319	0 0 0 0 0	

4637. $C_{57}H_{79}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1122.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.240E-04	3.636E-01	ns	B141	0 2 0 0 2	pH 7.5

4638. $C_{57}H_{79}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1122.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	4.602E-02	ns	B141	0 2 0 0 1	pH 7.5

4639. $C_{60}H_{77}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1156.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-04	3.966E-01	ns	B141	0 2 0 0 2	pH 7.5

4640. $C_{60}H_{92}N_{12}O_{10}$
Gramicidin S
Gramicidin
Cyclo(L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl-L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl)
Gramicidin S-A
RN: 113-73-5 **MP** (°C)**:**
MW: 1141.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-04	1.400E-01	28	A038	2 0 1 1 2	

4641. $C_{60}H_{98}N_{12}O_{37}S_{12}$
Dodecane(*S*-(carboxymethyl)-L-cystein))
RN: **MP** (°C)**:**
MW: 1964.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	4.518E-03	15	N331	0 0 0 0 0	
2.400E-05	4.714E-02	25	N331	0 0 0 0 0	
5.880E-05	1.155E-01	35	N331	0 0 0 0 0	

4642. $C_{60}H_{100}O_{50}$
6-*O*-α-D-Maltotriosyl-β-cyclodextrin
6-*O*-α-Maltotriosyl-β-cyclodextrin
6-*O*-α-D-Maltosyl-γ-cyclodextrin
6-*O*-α-Maltosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1621.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-01	1.524E+03	25	O321	0 0 0 0 0	
9.400E-01	1.524E+03	40	O321	0 0 0 0 0	
1.140E+00	1.848E+03	55	O321	0 0 0 0 0	
1.100E+00	1.784E+03	55	O321	0 0 0 0 0	

4643. $C_{62}H_{86}N_{12}O_{16}$
Actinomycin D
Actactinomycin A IV
Actinomycin AIV
Actinomycin I1
RN: 50-76-0 **MP** (°C)**:**
MW: 1255.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.983E-04	5.000E-01	37	G025	1 0 0 0 1	
7.965E-04	1.000E+00	rt	G025	0 0 0 0 1	

4644. $C_{62}H_{111}N_{11}O_{12}$
Cyclosporin A
1,4,7,10,13,16,19,22,25,28,31-Undecaazacyclotritriacontane, cyclic peptide deriv.
Sandimmun neoral
Sandimmun
Sang-35
SDZ-OXL 400
RN: 59865-13-3 **MP** (°C)**:** 148–151
MW: 1202.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.326E-05	4.000E-02	25	B376	0 0 0 0 0	
8.315E-06	1.000E-02	amb	L434	0 0 0 0 0	

4645. $C_{63}H_{85}N_{21}O_{19}$
Candicidin
Candeptin
Vanobid
RN: 1403-17-4 **MP** (°C)**:**
MW: 1440.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.349E-03	1.347E+01	21	M044	2 0 2 2 2	

4646. $C_{63}H_{88}N_{14}O_{14}PCo$
Vitamin B12
Cyanoject
Hydrobexan
Alphamine
Crystamine
Cyomin
RN: 68-19-9 **MP** (°C)**:**
MW: 1355.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.149E-03	1.240E+01	20	F300	1 0 0 0 2	

4647. $C_{64}H_{112}O_{40}$
Dimethyl-β-cyclodextrin
β-Cyclodextrin, 2A,2B,2C,2D,2E,2F,2G,6A,6B,6C,6D,6E,6F,6G-Tetradeca-*O*-methyl-
Heptakis(2,6-di-*O*-methyl)-β-cyclodextrin
Tetradeca-*O*-methyl-β-cyclodextrin
Tetradecakis-2,6-*O*-methylcycloheptaamylose
RN: 51166-71-3 **MP** (°C)**:** 298–300
MW: 1521.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	2.126E+02	c	D316	0 0 0 0 0	

4648. $C_{65}H_{106}N_{13}O_{40}S_{13}$
Tridecane(*S*-(carboxymethyl)-L-cyateine))
RN: **MP** (°C)**:**
MW: 2126.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.318E-02	25	N331	0 0 0 0 0	
1.600E-05	3.402E-02	35	N331	0 0 0 0 0	

4649. $C_{66}H_{84}O_{6}$
4-*tert*-Butylcalix[6]arene
5,11,17,23,29,35-Hexa-*tert*-butyl-37,38,39,40,41,42-hexahydroxycalix[6]arene
RN: 78092-53-2 **MP** (°C)**:** 380–381
MW: 973.40 **BP** (°C)**:** 890.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<9.73E-03	25	B424	1 0 1 2 2	

4650. $C_{66}H_{110}O_{55}$
6-*O*-α-D-Maltotriosyl-γ-cyclodextrin
6-*O*-α-Maltotriosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1783.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-01	1.516E+03	25	O321	0 0 0 0 0	
8.500E-01	1.516E+03	40	O321	0 0 0 0 0	
1.040E+00	1.855E+03	55	O321	0 0 0 0 0	

4651. $C_{67}H_{93}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1316.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.650E-04	4.806E-01	ns	B141	0 2 0 0 2	pH 7.5

4652. $C_{67}H_{93}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1316.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	4.937E-01	ns	B141	0 2 0 0 2	pH 7.5

4653. $C_{70}H_{89}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1348.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-04	3.021E-01	ns	B141	0 2 0 0 2	pH 7.5

4654. $C_{70}H_{126}O_{35}$
β-Cyclodextrin, tetradeca-*O*-ethyl-
Heptakis(2,6-di-*O*-ethyl)-β-cyclodextrin
RN: 194715-43-0 **MP** (°C)**:**
MW: 1527.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.273E-05	5.000E-02	25	H319	0 0 0 0 0	

4655. $C_{72}H_{85}N_{19}O_{18}S_5$
Thiostrepton
Bryamycin
RN: 1393-48-2 **MP** (°C)**:** 210
MW: 1664.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-05	8.800E-02	21	M044	2 0 2 2 1	
1.442E-04	2.400E-01	28	A038	2 0 1 1 1	

4656. $C_{72}H_{100}N_{18}O_{17}PCo$
Coenzyme B12
Cobamamide
Cobalamin, Co-(5′-deoxy-5′-adenosyl)-
Dibencozide
Funacomide
Deoxyadenosylcobalamin
RN: 13870-90-1 **MP** (°C)**:**
MW: 1579.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-02	2.600E+01	24	M054	1 0 0 0 1	

4657. $C_{74}H_{100}ClN_{15}O_{14}$
Antarelix
AcDNal-Dcpa-ser-tyr-dhai-leu-lys(ipr)-pro-dala-NH2
RN: 151272-78-5 **MP** (°C)**:**
MW: 1459.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.85E-03	>1.00E+01	ns	D350	0 1 0 1 1	

4658. $C_{75}H_{122}N_{15}O_{46}S_{15}$
Pendecane(*S*-(carboxymethyl)-L-cysteine))
RN: **MP** (°C)**:**
MW: 2450.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-07	8.333E-04	25	N331	0 0 0 0 0	

4659. $C_{77}H_{107}N_{17}O_{15}$
Pro-pro-pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1510.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-03	2.006E+00	ns	B141	0 2 0 0 2	pH 7.5

4660. $C_{80}H_{105}N_{17}O_{15}$

Pro-pro-pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr

RN: **MP** (°C)**:**

MW: 1544.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-04	1.298E+00	ns	B141	0 2 0 0 2	pH 7.5

4661. $C_{85}H_{117}N_{20}O_{18}$

Asp-arg-val-tyr-ile-his-pro-D-phe-his-leu-phe-val-tyr

RN: **MP** (°C)**:**

MW: 1707.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-05	1.058E-01	20	B141	1 2 0 0 1	pH 7.5

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Pharmaceutical Technology

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The **Handbook of Aqueous Solubility Data** gives scientists in a broad range of fields a portable, accessible resource for solubility data of numerous compounds and a single system for the evaluation of the data supplied.

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