Note: This is a reference cited in *AP 42, Compilation of Air Pollutant Emission Factors, Volume I Stationary Point and Area Sources.* AP42 is located on the EPA web site at www.epa.gov/ttn/chief/ap42/

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AP42 Section: 7.1

Background Chapter 3

Reference: 17

Title: **Henry's Law Constants for HAPs,**

Yaws, C.L.,

U. S. Environmental Protection Agency,
September 30, 1992.

FINAL REPORT

HENRY'S LAW CONSTANTS FOR HAP'S

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July 26, 1992

ABSTRACT

Results for Henry's law constant are presented for 109 organic chemicals in water. This represents major coverage of about 87.2 % (109/125 = 87.2 %) for the original listing of the 1990 Clean Air Act HAP'S. The results encompass representative values for most of the chemical families in the original list of HAP'S including aldehydes, amides, nitriles, ketones, acids, chlorides, anilines, benzenes, ethers, bromides, diolefins, disulfides, cresols, amines, oxides, ethylene glycols and others. The results for Henry's law constant at ambient conditions (25 C) are based on experimental (38 compounds), water solubility (22 compounds), VLE data (13 compounds) and UNIFAC (36 compounds).

For water solubility, experimental data are available for 58 compounds. This represents about 46.4 % coverage (58/125 = 46.4 %) for the original listing of the 1990 Clean Air Act HAP'S. A comparison (36 compounds) of experimental and calculated values using water solubility disclosed favorable agreement for Henry's law constant at ambient conditions (25 C).

In the absence of solubility and VLE (vapor-liquid equilibrium) data, values for compounds were estimated using UNIFAC (group contribution method). The UNIFAC method is based on group values (binary interaction and size parameters) for the molecular groups which are contained in compound. Most of the group values for UNIFAC are based on much simpler compounds than those contained in the HAP list. Also, most of the group values apply for compounds which are completely soluble in water. Many of the compounds in the HAP list contain benzene and other complex structures which are only partially soluble in water. Thus, the estimates should be considered as rough approximations.

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SECTION I

HENRY'S LAW CONSTANT

ABSTRACT

Results for Henry's law constant are presented for 109 organic chemicals in water. This represents major coverage of about 87.2 % (109/125 = 87.2 %) for the original listing of the 1990 Clean Air Act HAP'S. The results encompass representative values for most of the chemical families in the original list of HAP'S including aldehydes, amides, nitriles, ketones, acids, chlorides, anilines, benzenes, ethers, bromides, diolefins, disulfides, cresols, amines, oxides, ethylene glycols and others. The results for Henry's law constant at ambient conditions (25 C) are based on experimental (38 compounds), water solubility (22 compounds), VLE data (13 compounds) and UNIFAC (36 compounds).

HENRY'S LAW CONSTANT

Henry's law constant for a component in solution is applicable at very, very low concentrations. Since many such dilute aqueous solutions are encountered in industrial and environmental practice,Henry's law constant is especially important in environmental applications.

The results Henry's law constant for organic chemicals are given in Table 1. The tabulation is applicable to a wide variety of organic chemicals in contact with water at ambient conditions (25 C). The wide variety of chemicals includes aldehydes, amides, nitriles, ketones, acids, chlorides, anilines, benzenes, ethers, bromides, diolefins, disulfides, cresols, amines, oxides, ethylene glycols and others.

In Table 1, values for Henry's law constant are shown for EPA, CMA and the present work. The last column in the tabulation provides the basis (experimental, solubility, VLE data or UNIFAC) of the values for the present work.

Table 2 presents results of the present work in the various units used for Henry's law constant (atm/mol fraction, atm/mol/m^3, kPa/mol fraction and kPa/mol/m^3).

A comparison of experimental and calculated (using water solubility) values for Henry's law constant at ambient conditions (25 C) is shown in Figure 1. The graph includes data for many different organic chemicals (36 compounds). The graph discloses general agreement of experimental and calculated values.

EQUATIONS

Henry's law constant for a component in water may be determined from data for vapor pressure, water solubility and activity coefficient at infinite dilution (The derivation of the equations is provided in the Appendix). The thermodynamic equations are briefly summarized below:

LIQUIDS (PARTIAL SOLUBILITY)

$$H_i = \frac{1}{x_i} P_i^{SAT}$$

LIQUIDS (TOTAL SOLUBILITY)

$$H_i = \gamma_i^{\infty} P_i^{SAT}$$

GASES

$$H_i = (1-y_{H2O})/x_i$$

where H_i = Henry's law constant, atm/mol fraction

P_i^{SAT} = vapor pressure of organic chemical, atm

x_i = solubility of organic chemical in water, mol fraction

γ_i^{∞} = activity coefficient at infinite dilution

y_{H2O} = mol fraction of water in vapor phase at ambient conditions (at 25 C, y_{H2O} = 0.03117)

DISCUSSION

Experimental values for Henry's law constant at ambient conditions (25 C) are presented for 38 of the 125 organic compounds. This represents about 30.4 % coverage (38/125 = 30.4 %) of the original listing of the 1990 Clean Air Act HAP'S. The tabulated values for Henry's law constant are given in the Appendix of this report. A quick inspection of the tabulation discloses that there is general agreement of values among the several investigators. Examples of general agreement include benzene, carbon tetrachloride, chloroform, dichlorobenzene (1,4), ethylbenzene, ethyl chloride, ethylene dichloride, toluene and many others.

Tabulated values for vapor pressure are provided for 117 of the 125 organic compounds. Since 117/125 = 93.6 %, this represents appreciable major coverage of the organic compounds contained in the original listing of the 1990 Clean Air Act HAP'S. These tabulated values (see Appendix) provide results for vapor pressure as a function of temperature using an extended Antoine and Antoine equations. Using the provided correlation coefficients, the equations can be used to provide vapor pressure values at ambient (25 C) and other temperatures.

Experimental data for water solubility at ambient conditions (25 C) are presented for 58 of the 125 organic compounds. This represents about 46.4 % coverage (58/125 = 46.4 %) of the original listing of the 1990 Clean Air Act HAP'S. The tabulated values for water solubility are given in Appendix of this report. A quick inspection of the tabulation discloses that there is general agreement of values among most of the investigators. Examples of general agreement include acrylonitrile, benzene, carbon tetrachloride, chloroform, dichlorobenzene (1,4), hexane, ethylbenzene, ethylene dichloride, toluene and many others.

Results for activity coefficient at infinite dilution from VLE data (vapor-liquid equilibrium) are presented for 13 compounds. Unfortunately, this number is much lower than anticipated since VLE data could not be located for many of the compounds.

In the absence of data, values for 45 compounds were estimated using UNIFAC (group contribution

method). The UNIFAC method is based on group values (binary interaction and size parameters) for the molecular groups which are contained in compound. Most of the group values for UNIFAC are based on much simpler compounds than those contained in the HAP list. Also, most of the group values apply for compounds which are completely soluble in water. Many of the compounds in the HAP list contain benzene and other complex structures which are only partially soluble in water. Thus, the estimates should be considered as rough approximations.

The results for activity coefficient at infinite dilution cover 58 compounds (VLE data + estimates = 13 + 45 = 58) of the 125 organic compounds. This represents about 46.4 % coverage (58/125 = 46.4 %) of the original listing of the 1990 Clean Air Act HAP'S.The tabulated values for activity coefficient at infinite dilution are given in the Appendix of this report. For VLE data, a quick inspection of the tabulation discloses that there is general agreement of values among most of the investigators.

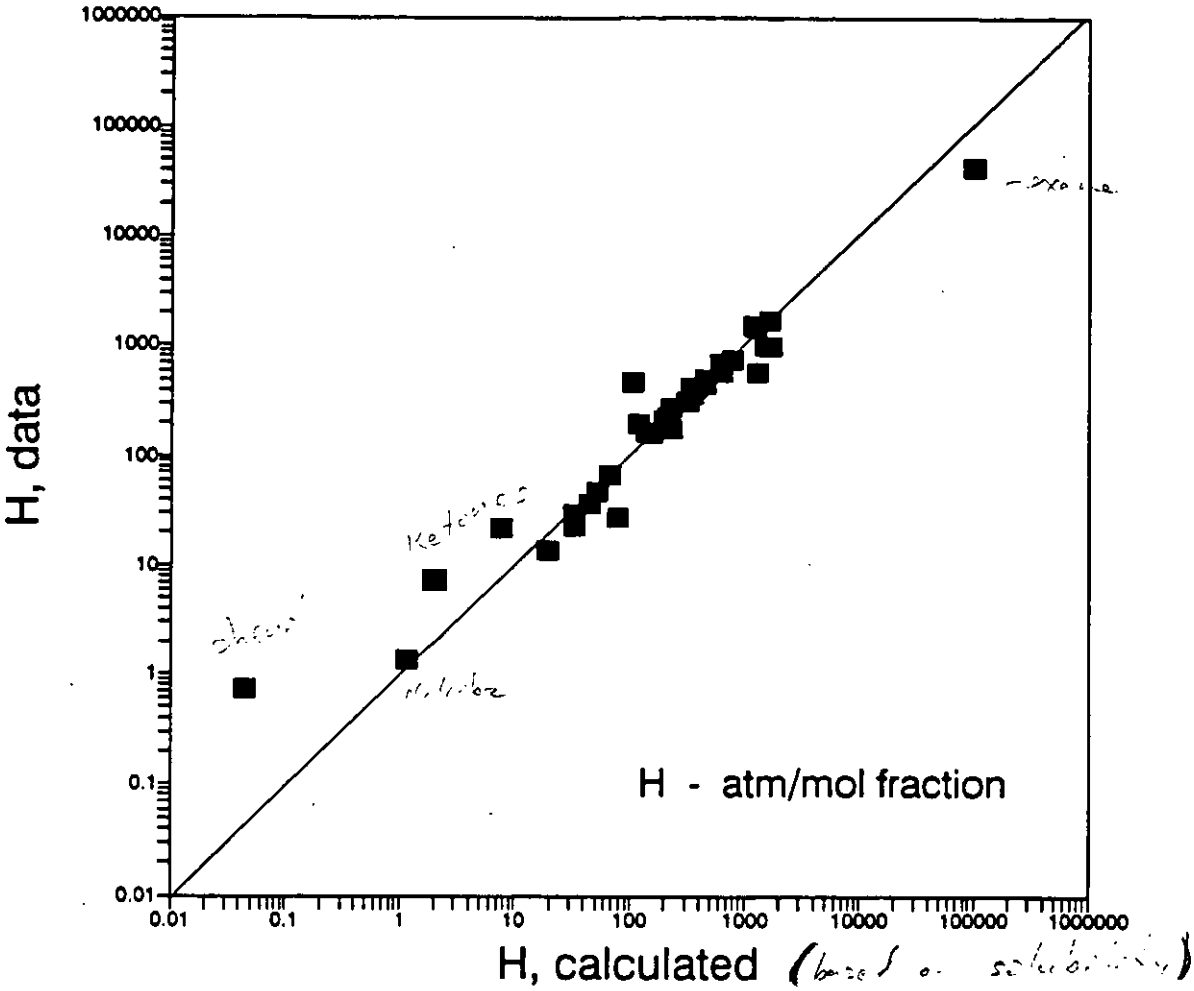

Figure 1 Henry's Law Constant

TABLE 1 HENRY'S LAW CONSTANT

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C (atm/mol fraction) EPA	CMA	PRESENT	BASIS
1	C2H4O	ACETALDEHYDE	5.27782	5.00560	6.51313	VLE DATA
2	C2H5ON	ACETAMIDE	0.07389	61.11160	0.00010	UNIFAC
3	C2H3N	ACETONITRILE	0.00322	1.11668	1.13641	VLE DATA
4	C8H8O	ACETOPHENONE	0.78334	0.58889	0.50894	SOLUBILITY
5	C3H4O	ACROLEIN	3.14447	2.44446	4.57118	SOLUBILITY
6	C3H5NO	ACRYLAMIDE	0.00003	0.00002	0.00001	UNIFAC
7	C3H4O2	ACRYLIC ACID	0.66667	0.01778	0.01107	VLE DATA
8	C3H3N	ACRYLONITRILE	4.88893	5.00004	5.44854	SOLUBILITY
9	C3H5CL	ALLYL CHLORIDE	20611.27600	266.11324	515.42218	SOLUBILITY
10	C6H7N	ANILINE	0.14445	0.43334	0.09776	SOLUBILITY
11	C7H9NO	O-ANISIDINE	45.55592	-------	0.00924	UNIFAC
12	C6H6	BENZENE	305.55800	240.00192	308.34000	EXPERIMENTAL
13	C7H5CL3	BENZOTRICHLORIDE	121.66764	-------	54.51771	UNIFAC
14	C7H7CL	BENZYL CHLORIDE	24.05575	19.16682	17.72868	UNIFAC
15	C12H10	BIPHENYL	5611.15600	35.33362	22.67000	EXPERIMENTAL
16	C2H4CL2O	BIS(CHLOROMETHYL)ETHER	11.66676	-------	5.02021	UNIFAC
17	CHBR3	BROMOFORM	32.44470	33.00026	29.56000	EXPERIMENTAL
18	C4H6	1,3-BUTADIENE	7888.95200	142778.92000	3961.17699	SOLUBILITY
19	C6H11ON	CAPROLACTAM	0.02528	0.01500	0.00016	UNIFAC
20	CS2	CARBON DISULFIDE	933.34080	1066.67520	1064.07986	SOLUBILITY
21	CCL4	CARBON TETRACHLORIDE	1666.68000	1288.89920	1677.79000	EXPERIMENTAL
22	C2H3CLO2	CHLOROACETIC ACID	0.00006	-------	0.00363	UNIFAC
23	C8H7CLO	2-CHLOROACETOPHENONE	13.33344	-------	-------	
24	C6H5CL	CHLOROBENZENE	218.33508	252.22424	209.45000	EXPERIMENTAL
25	CHCL3	CHLOROFORM	188.33484	203.89052	221.33000	EXPERIMENTAL
26	C4H5CL	CHLOROPRENE	18611.26000	161.11240	51.63556	UNIFAC
27	C7H8O	M-CRESOL	0.02461	0.04000	0.03948	SOLUBILITY
28	[redacted]	[redacted] CRESYLIC ACID [redacted]	1.18334	-------	-------	
29	C7H8O	O-CRESOL	0.14445	0.53000	0.09115	SOLUBILITY
30	C7H8O	P-CRESOL	0.02461	0.04200	0.03968	SOLUBILITY
31	C9H12	CUMENE	811.11760	800.00640	727.78000	EXPERIMENTAL
32	C6H4CL2	1,4-DICHLOROBENZENE	100.00080	240.55748	176.11000	EXPERIMENTAL
33	C4H8CL2O	DICHLOROETHYL ETHER	0.72223	63.88940	0.76435	UNIFAC
34	C3H4CL2	1,3-DICHLOROPROPENE*	129.44548	-------	197.22000	EXPERIMENTAL
35	C4H11NO2	DIETHANOLAMINE	406.11436	-------	-------	
36	C8H11N	N,N-DIMETYLANILINE	4.93337	4.44448	0.77013	UNIFAC
37	C4H10O4S	DIETHYL SULFATE	0.00756	-------	-------	
38	C14H20N	DIMETHYLBENZIDINE	24.44464	-------	-------	
39	C3H7NO	DIMETHYL FORMAMIDE	0.00019	-------	0.01061	VLE DATA
40	C2H8N2	1,1-DIMETHYLHYDRAZINE	6.88894	1388.90000	0.09108	VLE DATA
41	C10H10O4	DIMETHYL PHTHALATE	0.11945	0.00606	0.05485	UNIFAC
42	C2H6SO4	DIMETHYL SULFATE	0.03256	-------	-------	
43	C6H3N2O4	2,4-DINITROPHENOL	0.00850	-------	-------	
44	C7H6N2O4	2,4-DINITROTOLUENE	0.00001	-------	0.17227	UNIFAC
45	C4H8O2	1,4-DIOXANE	1.28334	0.41000	0.30647	VLE DATA
46	C12H12N2	1,2-DIPHENYLHYDRAZINE	194.44600	-------	-------	
47	C3H5CLO	EPICHLOROHYDRIN	1.79446	1.71112	0.44333	UNIFAC
48	C5H8O2	ETHYL ACRYLATE	19.44460	-------	5.65535	UNIFAC
49	C8H10	ETHYLBENZENE	357.78884	446.67024	437.81000	EXPERIMENTAL
50	C2H5CL	ETHYL CHLORIDE	505.55960	494.44840	672.23000	EXPERIMENTAL

TABLE 1 (CONTINUED)

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C (atm/mol fraction) EPA	CMA	PRESENT	BASIS
51	C2H4BR2	ETHYLENE DIBROMIDE	38.33364	-------	36.11000	EXPERIMENTAL
52	C2H4CL2	ETHYLENE DICHLORIDE	66.66720	-------	65.38000	EXPERIMENTAL
53	C2H6O2	ETHYLENE GLYCOL	0.00572	0.00012	0.00011	VLE DATA
54	C2H4O	ETHYLENE OXIDE	7.88895	4.35003	13.22808	VLE DATA
55	C2H4CL2	ETHYLIDENE DICHLORIDE	307.78024	-------	312.23000	EXPERIMENTAL
56	CH2O	FORMALDEHYDE	3.20003	0.01872	7.67602	UNIFAC
57	C4H10O2	ETHYLENE GLYCOL DIMETHYL ETHER	0.86112	2.10557	1.94713	VLE DATA
58	C4H10O2	ETHYLENE GLYCOL MONOETHYL ETHER	0.06167	0.05944	0.04797	VLE DATA
59	C8H16O4	DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE	0.01061	0.06056	0.03584	UNIFAC
60	C6H12O3	ETHYLENE GLYCOL MONOETHYL ETHER ACETATE	0.08278	0.45167	0.09862	SOLUBILITY
61	C6H14O3	DIETHYLENE GLYCOL MONOETHYL ETHER	0.00188	0.00260	0.00268	UNIFAC
62	C5H10O3	ETHYLENE GLYCOL MONOMETHYL ETHER ACETATE*	0.10833	0.33945	0.12187	UNIFAC
63	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL ETHER	0.00183	0.00203	0.00125	UNIFAC
64	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	0.00138	0.17167	0.08375	UNIFAC
65	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER	0.03833	0.04583	1716.68000	EXPERIMENTAL
66	C6H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	0.15222	0.08111	0.04742	UNIFAC
67	C8H10O2	ETHYLENE GLYCOL MONOPHENYL ETHER*	0.00274	0.00431	0.05604	SOLUBILITY
68	C5H12O2	DIETHYLENE GLYCOL MONOMETHYL ETHER	0.00126	0.00294	0.00226	UNIFAC
69	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	1.18334	0.19667	0.11892	UNIFAC
70	C6H14O2	ETHYLENE GLYCOL MONOBUTYL ETHER	0.04411	0.05539	0.02263	VLE DATA
71	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	0.02394	0.00498	0.00260	UNIFAC
72	C8H15O3	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE*	0.00058	0.44500	0.76245	SOLUBILITY
73	C6CL6	HEXACHLOROBENZENE	37.77808	71.11168	84.94337	SOLUBILITY
74	C4CL6	HEXACHLOROBUTADIENE	1433.34480	1277.78800	572.23000	EXPERIMENTAL
75	C2CL6	HEXACHLOROETHANE	0.13778	711.11680	463.89000	EXPERIMENTAL
76	C6H14	HEXANE	6777.83200	-------	42667.01000	EXPERIMENTAL
77	C8H6O2	HYDROQUINONE	8722.29200	-------	0.00002	UNIFAC
78	C9H14O	ISOPHORONE	0.32000	0.32000	2.19764	UNIFAC
79	C4H2O3	MALEIC ANHYDRIDE	0.00222	-------	0.01217	UNIFAC
80	CH4O	METHANOL	0.00150	0.15278	0.35648	VLE DATA
81	CH3BR	METHYL BROMIDE	12277.87600	11111.20000	381.06093	SOLUBILITY
82	CH3CL	METHYL CHLORIDE	452.22584	461.11480	490.00000	EXPERIMENTAL
83	C2H3CL3	METHYL CHLOROFORM	166.66800	-------	966.67000	EXPERIMENTAL
84	C4H8O	METHYL ETHYL KETONE	2.41669	3.18891	7.22000	EXPERIMENTAL
85	CH6N2	METHYL HYDRAZINE	0.19111	-------	0.02480	UNIFAC
86	C6H12O	METHYL ISOBUTYL KETONE	2.75002	7.61117	21.67000	EXPERIMENTAL
87	C2H3NO	METHYL ISOCYANATE	1.26668	-------	-------	
88	C5H8O2	METHYL METHACRYLATE	3.66670	17.77792	4.72284	UNIFAC
89	C5H12O	METHYL TERT-BUTYL ETHER	278.33556	27.00022	30.84043	SOLUBILITY
90	CH2CL2	METHYLENE CHLORIDE	177.22364	113.33424	164.45000	EXPERIMENTAL
91	C15H10N2O2	METHYLENE DIPHENYL DIISOCYANATE	297.22460	-------	-------	
92	C13H14N2	4,4-METHYLENEDIANILINE	0.15556	-------	-------	
93	C10H8	NAPHTHALENE	65.55608	26.22243	26.83000	EXPERIMENTAL
94	C6H5NO2	NITROBENZENE	0.72778	1.31668	1.33000	EXPERIMENTAL
95	C6H5NO3	4-NITROPHENOL	0.03939	0.00181	-------	
96	C3H7NO2	2-NITROPROPANE	67.22276	-------	6.61124	SOLUBILITY
97	C6H6O	PHENOL	0.02522	0.02594	0.72200	EXPERIMENTAL
98	C6H8N2	P-PHENYLENEDIAMINE	0.00063	-------	0.00007	UNIFAC
99	COCL2	PHOSGENE	9500.07600	11000.08800	4400.00000	
100	C8H4O3	PHTHALIC ANHYDRIDE	0.05000	0.00034	0.00784	UNIFAC

TABLE 1 (CONTINUED)

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C (atm/mol fraction) EPA	CMA	PRESENT	BASIS
101	C3H4O2	BETA-PROPIOLACTONE	0.05122	-------	0.00638	UNIFAC
102	C3H6O	PROPIONALDEHYDE	56389.34000	6.38894	3.32252	SOLUBILITY
103	C3H6CL2	PROPYLENE DICHLORIDE	127.77880	150.00120	158.71000	EXPERIMENTAL
104	C3H6O	PROPYLENE OXIDE	74.44504	20.00016	19.77430	VLE DATA
105	C6H4O2	QUINONE	400.00320	0.04778	-------	.05 B
106	C8H8	STYRENE	183.33480	146.11228	144.71670	SOLUBILITY
107	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	21.11128	-------	13.89000	EXPERIMENTAL
108	C2CL4	TETRACHLOROETHYLENE	1594.45720	983.34120	983.34000	EXPERIMENTAL
109	C7H8	TOLUENE	381.11416	255.55760	356.67000	EXPERIMENTAL
110	C7H10N2	2,4-TOLUENE DIAMINE	0.33500	-------	0.00007	UNIFAC
111	C9H6N2O2	2,4-TOLUENE DIISOCYANATE	0.46111	-------	-------	
112	C7H9N	O-TOLUIDINE	1.06112	-------	0.10457	UNIFAC
113	C6H3CL3	1,2,4-TRICHLOROBENZENE	78.88952	160.00128	106.67000	EXPERIMENTAL
114	C2H3CL3	1,1,2-TRICHLOROETHANE	41.11144	-------	45.77000	EXPERIMENTAL
115	C2HCL3	TRICHLROETHYLENE	505.55960	532.22648	566.67000	EXPERIMENTAL
116	C6H3CL3O	2,4,5-TRICHLOROPHENOL	0.98334	1.10001	0.03520	UNIFAC
117	C6H15N	TRIETHYLAMINE	147.77896	8.11118	6.94285	SOLUBILITY
118	C8H18	2,2,4-TRIMETHYLPENTANE	133.88996	175001.40000	185452.92157	SOLUBILITY
119	C4H6O2	VINYL ACETATE	34.44472	26.88910	28.21141	SOLUBILITY
120	C2H3CL	VINYL CHLORIDE	4722.26000	4661.14840	1472.23000	EXPERIMENTAL
121	C2H2CL2	VINYLIDENE CHLORIDE	833.34000	1450.01160	1438.90000	EXPERIMENTAL
~~122~~		~~XYLENES (ISOMERS & MIXTURES)~~	~~288.89120~~	-------	-------	
123	C8H10	M-XYLENE	292.78012	410.00328	413.34000	EXPERIMENTAL
124	C8H10	O-XYLENE	292.78012	290.00232	270.56000	EXPERIMENTAL
125	C8H10	P-XYLENE	292.78012	370.00296	413.34000	EXPERIMENTAL

* - Estimated values for coefficients in vapor pressure equation.

why isn't 2,4,6 trichlorophenol on list

TABLE 2 HENRY'S LAW CONSTANT - ATM AND KPA UNITS

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C			
			atm/mol fra	atm/mol/m^3	kPa/mol fra	kPa/mol/m^3
1	C2H4O	ACETALDEHYDE	6.51313	1.172E-04	659.943	1.188E+01
2	C2H5ON	ACETAMIDE	0.00010	1.800E-09	0.010	1.824E-04
3	C2H3N	ACETONITRILE	1.13641	2.046E-05	115.147	2.073E+00
4	C8H8O	ACETOPHENONE	0.50894	9.161E-06	51.568	9.282E-01
5	C3H4O	ACROLEIN	4.57118	8.228E-05	463.175	8.337E+00
6	C3H5NO	ACRYLAMIDE	0.00001	1.800E-10	0.001	1.824E-05
7	C3H4O2	ACRYLIC ACID	0.01107	1.993E-07	1.122	2.019E-02
8	C3H3N	ACRYLONITRILE	5.44854	9.807E-05	552.073	9.937E+00
9	C3H5CL	ALLYL CHLORIDE	515.42218	9.278E-03	52225.152	9.400E+02
10	C6H7N	ANILINE	0.09776	1.760E-06	9.906	1.783E-01
11	C7H9NO	O-ANISIDINE	0.00924	1.663E-07	0.936	1.685E-02
12	C6H6	BENZENE	308.34000	5.550E-03	31242.550	5.624E+02
13	C7H5CL3	BENZOTRICHLORIDE	54.51771	9.813E-04	5524.007	9.943E+01
14	C7H7CL	BENZYL CHLORIDE	17.72868	3.191E-04	1796.359	3.233E+01
15	C12H10	BIPHENYL	22.67000	4.081E-04	2297.038	4.135E+01
16	C2H4CL2O	BIS(CHLOROMETHYL)ETHER	5.02021	9.036E-05	508.673	9.156E+00
17	CHBR3	BROMOFORM	29.56000	5.321E-04	2995.167	5.391E+01
18	C4H6	1,3-BUTADIENE	3961.17699	7.130E-02	401366.259	7.225E+03
19	C6H11ON	CAPROLACTAM	0.00016	2.880E-09	0.016	2.918E-04
20	CS2	CARBON DISULFIDE	1064.07986	1.915E-02	107817.892	1.941E+03
21	CCL4	CARBON TETRACHLORIDE	1677.79000	3.020E-02	170002.072	3.060E+03
22	C2H3CLO2	CHLOROACETIC ACID	0.00363	6.534E-08	0.368	6.621E-03
23	C8H7CLO	2-CHLOROACETOPHENONE	-------	---------	-----	---------
24	C6H5CL	CHLOROBENZENE	209.45000	3.770E-03	21222.521	3.820E+02
25	CHCL3	CHLOROFORM	221.33000	3.984E-03	22426.262	4.037E+02
26	C4H5CL	CHLOROPRENE	51.63556	9.294E-04	5231.973	9.417E+01
27	C7H8O	M-CRESOL	0.03948	7.106E-07	4.000	7.201E-02
28		CRESOLS/CRESYLIC ACID(ISOMERS & MIXTURES)	-------	---------	-----	---------
29	C7H8O	O-CRESOL	0.09115	1.641E-06	9.236	1.662E-01
30	C7H8O	P-CRESOL	0.03968	7.142E-07	4.021	7.237E-02
31	C9H12	CUMENE	727.78000	1.310E-02	73742.308	1.327E+03
32	C6H4CL2	1,4-DICHLOROBENZENE	176.11000	3.170E-03	17844.346	3.212E+02
33	C4H8CL2O	DICHLOROETHYL ETHER	0.76435	1.376E-05	77.448	1.394E+00
34	C3H4CL2	1,3-DICHLOROPROPENE*	197.22000	3.550E-03	19983.317	3.597E+02
35	C4H11NO2	DIETHANOLAMINE	-------	---------	-----	---------
36	C8H11N	N,N-DIMETYLANILINE	0.77013	1.386E-05	78.033	1.405E+00
37	C4H10O4S	DIETHYL SULFATE	-------	---------	-----	---------
38	C14H20N	DIMETHYLBENZIDINE	-------	---------	-----	---------
39	C3H7NO	DIMETHYL FORMAMIDE	0.01061	1.910E-07	1.075	1.935E-02
40	C2H8N2	1,1-DIMETHYLHYDRAZINE	0.09108	1.639E-06	9.229	1.661E-01
41	C10H10O4	DIMETHYL PHTHALATE	0.05485	9.873E-07	5.558	1.000E-01
42	C2H6SO4	DIMETHYL SULFATE	-------	---------	-----	---------
43	C6H3N2O4	2,4-DINITROPHENOL	-------	---------	-----	---------
44	C7H6N2O4	2,4-DINITROTOLUENE	0.17227	3.101E-06	17.455	3.142E-01
45	C4H8O2	1,4-DIOXANE	0.30647	5.516E-06	31.053	5.590E-01
46	C12H12N2	1,2-DIPHENYLHYDRAZINE	-------	---------	-----	---------
47	C3H5CLO	EPICHLOROHYDRIN	0.44333	7.980E-06	44.920	8.086E-01
48	C5H8O2	ETHYL ACRYLATE	5.65535	1.018E-04	573.028	1.031E+01
49	C8H10	ETHYLBENZENE	437.81000	7.881E-03	44361.098	7.985E+02
50	C2H5CL	ETHYL CHLORIDE	672.23000	1.210E-02	68113.705	1.226E+03

1.86 (9/30/93)

TABLE 2 (CONTINUED)

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C			
			atm/mol fra	atm/mol/m^3	kPa/mol fra	kPa/mol/m^3
51	C2H4BR2	ETHYLENE DIBROMIDE	36.11000	6.500E-04	3658.846	6.586E+01
52	C2H4CL2	ETHYLENE DICHLORIDE	65.38000	1.177E-03	6624.628	1.192E+02
53	C2H6O2	ETHYLENE GLYCOL	0.00011	1.980E-09	0.011	2.006E-04
54	C2H4O	ETHYLENE OXIDE	13.22808	2.381E-04	1340.335	2.413E+01
55	C2H4CL2	ETHYLIDENE DICHLORIDE	312.23000	5.620E-03	31636.705	5.695E+02
56	CH2O	FORMALDEHYDE	7.67602	1.382E-04	777.773	1.400E+01
57	C4H10O2	ETHYLENE GLYCOL DIMETHYL ETHER	1.94713	3.505E-05	197.293	3.551E+00
58	C4H10O2	ETHYLENE GLYCOL MONOETHYL ETHER	0.04797	8.635E-07	4.861	8.749E-02
59	C8H16O4	DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE	0.03584	6.451E-07	3.631	6.537E-02
60	C6H12O3	ETHYLENE GLYCOL MONOETHYL ETHER ACETATE	0.09862	1.775E-06	9.993	1.799E-01
61	C6H14O3	DIETHYLENE GLYCOL MONOETHYL ETHER	0.00268	4.824E-08	0.272	4.888E-03
62	C5H10O3	ETHYLENE GLYCOL MONOMETHYL ETHER ACETATE*	0.12187	2.194E-06	12.348	2.223E-01
63	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL ETHER	0.00125	2.250E-08	0.127	2.280E-03
64	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	0.08375	1.507E-06	8.486	1.527E-01
65	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER	1716.68000	3.090E-02	173942.601	3.131E+03
66	C6H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	0.04742	8.536E-07	4.805	8.649E-02
67	C8H10O2	ETHYLENE GLYCOL MONOPHENYL ETHER*	0.05604	1.009E-06	5.678	1.022E-01
68	C5H12O2	DIETHYLENE GLYCOL MONOMETHYL ETHER	0.00226	4.068E-08	0.229	4.122E-03
69	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	0.11892	2.141E-06	12.050	2.169E-01
70	C6H14O2	ETHYLENE GLYCOL MONOBUTYL ETHER	0.02263	4.073E-07	2.293	4.127E-02
71	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	0.00260	4.680E-08	0.263	4.742E-03
72	C8H15O3	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE*	0.76245	1.372E-05	77.255	1.391E+00
73	C6CL6	HEXACHLOROBENZENE	84.94337	1.529E-03	8606.887	1.549E+02
74	C4CL6	HEXACHLOROBUTADIENE	572.23000	1.030E-02	57981.205	1.044E+03
75	C2CL6	HEXACHLOROETHANE	463.89000	8.350E-03	47003.654	8.461E+02
76	C6H14	HEXANE	42667.01000	7.680E-01	4323234.788	7.782E+04
77	C8H6O2	HYDROQUINONE	0.00002	3.600E-10	0.002	3.648E-05
78	C9H14O	ISOPHORONE	2.19764	3.956E-05	222.676	4.008E+00
79	C4H2O3	MALEIC ANHYDRIDE	0.01217	2.191E-07	1.233	2.220E-02
80	CH4O	METHANOL	0.35648	6.417E-06	36.120	6.502E-01
81	CH3BR	METHYL BROMIDE	381.06093	6.859E-03	38610.999	6.950E+02
82	CH3CL	METHYL CHLORIDE	49-------	8.820E-03	49649.250	8.937E+02
83	C2H3CL3	METHYL CHLOROFORM	966.67000	1.740E-02	97947.838	1.763E+03
84	C4H8O	METHYL ETHYL KETONE	7.22000	1.300E-04	731.567	1.317E+01
85	CH6N2	METHYL HYDRAZINE	0.02480	4.464E-07	2.513	4.523E-02
86	C6H12O	METHYL ISOBUTYL KETONE	21.67000	3.901E-04	2195.713	3.952E+01
87	C2H3NO	METHYL ISOCYANATE	-------	---------	-----	---------
88	C5H8O2	METHYL METHACRYLATE	4.72284	8.501E-05	478.542	8.614E+00
89	C5H12O	METHYL TERT-BUTYL ETHER	30.84043	5.551E-04	3124.907	5.625E+01
90	CH2CL2	METHYLENE CHLORIDE	164.45000	2.960E-03	16662.896	2.999E+02
91	C15H10N2O2	METHYLENE DIPHENYL DIISOCYANATE	-------	---------	-----	---------
92	C13H14N2	4,4-METHYLENEDIANILINE	-------	---------	-----	---------
93	C10H8	NAPHTHALENE	26.83000	4.829E-04	2718.550	4.893E+01
94	C6H5NO2	NITROBENZENE	1.33000	2.394E-05	134.762	2.426E+00
95	C6H5NO3	4-NITROPHENOL	-------	---------	-----	---------
96	C3H7NO2	2-NITROPROPANE	6.61124	1.190E-04	669.884	1.206E+01
97	C6H6O	PHENOL	0.72200	1.300E-05	73.157	1.317E+00
98	C6H8N2	P-PHENYLENEDIAMINE	0.00007	1.260E-09	0.007	1.277E-04
99	COCL2	PHOSGENE	-------	---------	-----	---------
100	C8H4O3	PHTHALIC ANHYDRIDE	0.00784	1.411E-07	0.794	1.430E-02

TABLE 2 (CONTINUED)

NO	FORMULA	NAME	Henry's Law Constant, H @ 25 C			
			atm/mol fra	atm/mol/m^3	kPa/mol fra	kPa/mol/m^3
101	C3H4O2	BETA-PROPIOLACTONE	0.00638	1.148E-07	0.646	1.164E-02
102	C3H6O	PROPIONALDEHYDE	3.32252	5.980E-05	336.654	6.060E+00
103	C3H6CL2	PROPYLENE DICHLORIDE	158.71000	2.857E-03	16081.291	2.895E+02
104	C3H6O	PROPYLENE OXIDE	19.77430	3.559E-04	2003.631	3.607E+01
105	C6H4O2	QUINONE	-------	---------	-----	---------
106	C8H8	STYRENE	144.71670	2.605E-03	14663.420	2.639E+02
107	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	13.89000	2.500E-04	1407.404	2.533E+01
108	C2CL4	TETRACHLOROETHYLENE	983.34000	1.770E-02	99636.926	1.793E+03
109	C7H8	TOLUENE	356.67000	6.420E-03	36139.588	6.505E+02
110	C7H10N2	2,4-TOLUENE DIAMINE	0.00007	1.260E-09	0.007	1.277E-04
111	C9H6N2O2	2,4-TOLUENE DIISOCYANATE	-------	---------	-----	---------
112	C7H9N	O-TOLUIDINE	0.10457	1.882E-06	10.596	1.907E-01
113	C6H3CL3	1,2,4-TRICHLOROBENZENE	106.67000	1.920E-03	10808.338	1.945E+02
114	C2H3CL3	1,1,2-TRICHLOROETHANE	45.77000	8.239E-04	4637.645	8.348E+01
115	C2HCL3	TRICHLROETHYLENE	566.67000	1.020E-02	57417.838	1.034E+03
116	C6H3CL3O	2,4,5-TRICHLOROPHENOL	0.03520	6.336E-07	3.567	6.420E-02
117	C6H15N	TRIETHYLAMINE	6.94285	1.250E-04	703.484	1.266E+01
118	C8H18	2,2,4-TRIMETHYLPENTANE	185452.92157	3.338E+00	18791017.280	3.382E+05
119	C4H6O2	VINYL ACETATE	28.21141	5.078E-04	2858.521	5.145E+01
120	C2H3CL	VINYL CHLORIDE	1472.23000	2.650E-02	149173.705	2.685E+03
121	C2H2CL2	VINYLIDENE CHLORIDE	1438.90000	2.590E-02	145796.543	2.624E+03
122		XYLENES (ISOMERS & MIXTURES)	-------	---------	-----	---------
123	C8H10	M-XYLENE	413.34000	7.440E-03	41881.675	7.539E+02
124	C8H10	O-XYLENE	270.56000	4.870E-03	27414.492	4.935E+02
125	C8H10	P-XYLENE	413.34000	7.440E-03	41881.675	7.539E+02

• - Estimated values for coefficients in vapor pressure equation.
mol fra - mol fraction

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APPENDIX A

HENRY'S LAW CONSTANT - EQUATIONS

The calculation of Henry's law constant for a component in water may be achieved using data for solubility, vapor pressure and activity coefficient at infinite dilution. Derivation of the equations is briefly given in the following discussion.

LIQUIDS (PARTIAL SOLUBILITY)

For organic chemicals which are liquids at ambient conditions and have partial solubility in water, there are three phases when the organic chemical is in contact with water. These are vapor, organic and water phases. Such a three phase system consisting of vapor, liquid I and liquid II is shown in Fig. A-1a. At equilibrium, the fugacity of the component in each liquid phase is given by:

$$f_i^{liq\ I} = f_i^{liq\ II} \qquad \text{(A-1)}$$

For the organic phase (liquid I), the fugacity of the component is: γ_i * mol fraction$_i$ * vapor pressure$_i$ (where γ_i is the activity coefficient). Since the organic phase has only very small concentration of water (ppm level or less), the mol fraction of the organic chemical is approximately equal to 1 (mol fraction$_i$=1). This is also true for the activity coefficient of the organic chemical (γ_i=1). Thus

$$f_i^{liq\ I} = P_i^{SAT} \qquad \text{(A-2)}$$

For the water phase (liquid II), the fugacity of the component is given by Henry's law which is applicable at very small concentration:

$$f_i^{liq\ II} = H_i\, x_i^{liq\ II} \qquad (x_i << 1) \qquad \text{(A-3)}$$

Substitution of equations (A-2) and (A-3) into equation (A-1) yields:

$$P_i^{SAT} = H_i\, x_i^{liq\ II} \qquad \text{(A-4)}$$

Solving for Henry's law constant yields the following equation which is applicable to organic chemicals which are liquids at ambient conditions (25 C, 1 atm) and have only small partial solubility in water:

$$H_i = \frac{1}{x_i^{liq\ II}}\, P_i^{SAT} \qquad \text{(A-5)}$$

where H_i = Henry's law constant, atm/mol fraction

$x_i^{liq\ II}$ = solubility of organic chemical in water, mol fraction

P_i^{SAT} = vapor pressure of organic chemical, atm

LIQUIDS (TOTAL SOLUBILITY)

For organic chemicals which are liquids at ambient conditions and have total solubility in water, there are two phases when the organic chemical is in contact with water. These are vapor and liquid phases. Fig. A-1b shows such a two phase system.

For the liquid phase, the fugacity of the organic chemical is: γ_i • mol fraction$_i$ • vapor pressure$_i$ (where γ_i is the activity coefficient). Since the liquid phase has only very small concentration of organic chemical (ppm level or less) in the region where Henry's law is applicable, the activity coefficient is the activity coefficient at infinite dilution ($\gamma_i = \gamma_i^{\infty}$). Thus

$$f_i^{liq} = \gamma_i^{\infty} x_i P_i^{SAT} \qquad \text{(A-6)}$$

For the liquid phase, the fugacity of the component is given by Henry's law which is applicable at very small concentration:

$$f_i^{liq} = H_i x_i \qquad (x_i << 1) \qquad \text{(A-7)}$$

Substitution of equation (A-6) into equation (A-7) yields:

$$\gamma_i^{\infty} x_i P_i^{SAT} = H_i x_i \qquad \text{(A-8)}$$

Solving for Henry's law constant yields the following equation which is applicable to organic chemicals which are liquids at ambient conditions (25 C, 1 atm) and have total solubility in water:

$$H_i = \gamma_i^{\infty} P_i^{SAT} \qquad \text{(A-9)}$$

where H_i = Henry's law constant, atm/mol fraction

γ_i^{∞} = activity coefficient at infinite dilution

P_i^{SAT} = vapor pressure of organic chemical, atm

GASES

For organic chemicals which are gases at ambient conditions, there are two phases when the organic chemical is in contact with water. These are vapor and liquid phases. Such a two phase system consisting of vapor and liquid is shown in Fig. A-1b. At equilibrium, the fugacity of the component in each phase is given by:

$$f_i^{vap} = f_i^{liq} \qquad \text{(A-10)}$$

For the vapor phase, the fugacity of the organic chemical is:

$$f_i^{vap} = y_i P_t \qquad \text{(A-11)}$$

Substitution of $y_i = 1\text{-}y_{H2O}$ and $P_t = 1$ atm into the equation provides:

$$f_i^{vap} = 1\text{-}y_{H2O} \qquad \text{(A-12)}$$

For the liquid phase, the fugacity of the component is given by Henry's law which is applicable at very small concentration:

$$f_i^{liq} = H_i x_i \qquad (x_i << 1) \tag{A-13}$$

Substitution of equations (A-12) and (A-13) into equation (A-10) yields:

$$1-y_{H2O} = H_i x_i \tag{A-14}$$

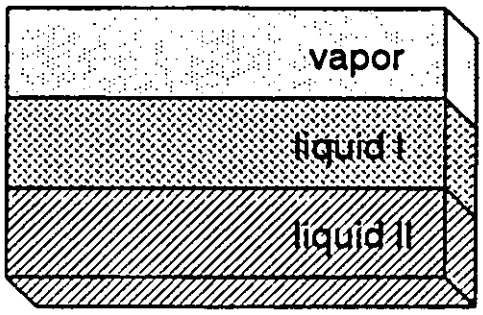
Solving for Henry's law constant yields the following equation which is applicable to organic chemicals which are gases at ambient conditions (25 C, 1 atm):

$$H_i = (1-y_{H2O})/x_i \tag{A-15}$$

where H_i = Henry's law constant, atm/mol fraction

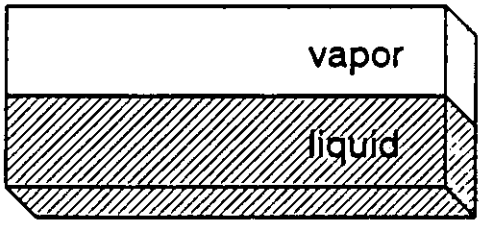
x_i = solubility of organic chemical in water, mol fraction

y_{H2O} = mol fraction of water in vapor phase at ambient conditions (at 25 C, y_{H2O} = 0.03117)



$$fi^{vap} = fi^{liq\ I} = fi^{liq\ II}$$

Fig.A-1a Three phase system



$$fi^{vap} = fi^{liq}$$

Fig. A-1b Two phase system

APPENDIX B

CONVERSION FACTORS FOR HENRY'S LAW CONSTANT

The units for Henry's law constant which is applicable at very, very low concentration involve pressure and concentration. Since there are several ways to express pressure and concentration, it is often necessary to convert values for Henry's law constant. The following factors are helpful in the conversions:

To convert from H in atm/mol fraction to:

H in atm/(mol/m^3), divide by 55,556

H in mm Hg/mol fraction, multiply by 760

H in psia/mol fraction, multiply by 14.7

H in kPa/mol fraction, multiply by 101.325

H in kPa/(mol/m^3), multipy by 101.325/55,556

APPENDIX C

HENRY'S LAW CONSTANT - EXPERIMENTAL VALUES

No	Formula	Name	Henry's Law Constant in Water @ 25 C atm/mol frac	Source
12	C6H6	BENZENE	308.34	Selected
			293.34	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			308.34	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			306.34	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
			308.34	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
15	C12H10	BIPHENYL	22.67	Selected
			22.67	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
17	CHBR3	BROMOFORM	29.56	Selected
			29.56	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
21	CCL4	CARBON TETRACHLORIDE	1677.79	Selected
			1816.68	Zhou, Z., HENRY'S LAW CONSTANT OF VOLATILE ORGANIC COMPOUNDS, MS thesis, Lamar Univ., (1990).
			1638.90	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			1688.90	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			1677.79	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			1532.84	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
24	C6H5CL	CHLOROBENZENE	209.45	Selected
			144.45	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			218.34	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).

			182.18	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
			209.45	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
25	CHCL3	CHLOROFORM	221.33	Selected
			233.89	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			203.89	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			188.34	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			221.33	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
31	C9H12	CUMENE	727.78	Selected
			727.78	Zhou, Z., HENRY'S LAW CONSTANT OF VOLATILE ORGANIC COMPOUNDS, MS thesis, Lamar Univ., (1990).
32	C6H4CL2	1,4-DICHLOROBENZENE	176.11	Selected
			176.11	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			151.11	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
34	C3H4CL2	1,3-DICHLOROPROPENE	197.22	Selected
			197.22	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
49	C8H10	ETHYLBENZENE	437.81	Selected
			437.81	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			357.78	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			468.34	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
50	C2H5CL	ETHYL CHLORIDE	672.23	Selected
			672.23	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			616.67	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
51	C2H4BR2	ETHYLENE BROMIDE	36.11	Selected

			36.11	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
52	C2H4CL2	ETHYLENE DICHLORIDE	65.38	Selected
			78.33	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			61.11	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			65.38	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
55	C2H4CL2	ETHYLIDENE DICHLORIDE	312.23	Selected
			347.23	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			312.23	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			302.78	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
65	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER	1716.68	Selected
			1716.68	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
73	C6CL6	HEXACHLOROBENZENE	94.45	Selected
			94.45	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
74	C4CL6	HEXACHLOROBUTADIENE	572.23	Selected
			572.23	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
75	C2CL6	HEXACHLOROETHANE	463.89	Selected
			463.89	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			547.23	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
76	C6H14	HEXANE	42667.01	Selected
			42667.01	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
82	CH3CL	METHYL CHLORIDE	490.00	Selected
			490.00	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
83	C2H3CL3	METHYL CHLOROFORM	966.67	Selected

			966.67	Zhou, Z., HENRY'S LAW CONSTANT OF VOLATILE ORGANIC COMPOUNDS, MS thesis, Lamar Univ., (1990).
			966.67	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			955.56	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			273.34	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			1103.43	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
84	C4H8O	METHYL ETHYL KETONE	7.22	Selected
			7.22	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
86	C6H12O	METHYL ISOBUTYL KETONE	21.67	Selected
			21.67	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
90	CH2CL2	METHYLENE CHLORIDE	164.45	Selected
			164.45	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			121.67	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			177.22	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			180.30	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
93	C10H8	NAPHTHALENE	26.83	Selected
			26.83	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
94	C6H5NO2	NITROBENZENE	1.333	Selected
			1.333	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
97	C6H6O	PHENOL	0.722	Selected
			0.722	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
103	C3H6CL2	PROPYLENE DICHLORIDE	158.71	Selected
			158.71	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
107	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	13.89	Selected

			13.89	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			20.36	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
108	C2CL4	TETRACHLOROETHYLENE	983.34	Selected
			950.01	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			983.34	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			1594.46	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			896.71	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
109	C7H8	TOLUENE	356.67	Selected
			356.67	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			329.45	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			357.48	Leighton, D. T. and J. M. Calo, J. Chem. Eng. Data, 26, 382 (1981).
			368.89	Mackay, D., W. Y. Shiu and R. P. Sutherland, Environ. Sci. Technol., 13, 333 (1979).
113	C6H3CL3	1,2,4-TRICHLOROBENZENE	106.67	Selected
			106.67	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			78.89	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
114	C2H3CL3	1,1,2-TRICHLOROETHANE	45.77	Selected
			45.11	Zhou, Z., HENRY'S LAW CONSTANT OF VOLATILE ORGANIC COMPOUNDS, MS thesis, Lamar Univ., (1990).
			50.56	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			45.77	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
115	C2HCL3	TRICHLROETHYLENE	566.67	Selected
			566.67	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			532.27	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).

			650.01	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			546.69	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
120	C2H3CL	VINYL CHLORIDE	1472.23	Selected
			1472.23	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			1544.46	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
121	C2H2CL2	VINYLIDENE CHLORIDE	1438.90	Selected
			1438.90	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
			1450.01	Gossett, J. M., Environ. Sci. Technol., 21, 202 (1987).
			833.34	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
			2061.42	Warner, H. P., J. C. Cohen and J. C. Ireland, EPA/600/D-87/229, US EPA, Cincinnati, OH (1987).
123	C8H10	M-XYLENE	413.34	Selected
			413.34	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
124	C8H10	O-XYLENE	270.56	Selected
			270.56	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).
125	C8H10	P-XYLENE	413.34	Selected
			469.45	Zhou, Z., HENRY'S LAW CONSTANT OF VOLATILE ORGANIC COMPOUNDS, MS thesis, Lamar Univ., (1990).
			413.34	Ashworth, R. A., G. W. Howe, M. E. Mullins and T. E. Rogers, J. of Hazardous Materials, 18, 25 (1988).

APPENDIX D

TABLE D-1 VAPOR PRESSURE - EXTENDED ANTOINE EQUATION

$\ln P = A + B/T + C \ln T + D T^E$ (P - mm Hg, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
1	C2H4O	ACETALDEHYDE	201.1772	-8.4786E+03	-3.1548E+01	4.6314E-02	1	150.15	461.00
2	C2H5ON	ACETAMIDE	127.5872	-1.1961E+04	-1.6068E+01	1.1880E-05	2	354.15	494.30
3	C2H3N	ACETONITRILE	53.4092	-5.3856E+03	-5.4954E+00	5.3634E-06	2	229.32	545.50
4	C8H8O	ACETOPHENONE	127.9772	-1.0385E+04	-1.7284E+01	1.4779E-02	1	292.80	701.00
5	C3H4O	ACROLEIN	133.5072	-7.1227E+03	-1.9638E+01	2.6447E-02	1	185.45	506.00
6	C3H5NO	ACRYLAMIDE	39.1412	-1.0231E+04	-1.7139E+00	----	-	357.65	465.75
7	C3H4O2	ACRYLIC ACID	53.0992	-7.2180E+03	-4.8813E+00	1.0060E-03	1	286.65	615.00
8	C3H3N	ACRYLONITRILE	82.7112	-6.3927E+03	-1.0101E+01	1.0891E-05	2	186.63	535.00
9	C3H5CL	ALLYL CHLORIDE	38.1982	-4.3084E+03	-3.1322E+00	1.1171E-17	6	138.65	514.15
10	C6H7N	ANILINE	286.3872	-1.6504E+04	-4.2763E+01	3.9918E-02	1	267.13	699.00
11	C7H9NO	O-ANISIDINE	----	----	----	----	-	---	---
12	C6H6	BENZENE	73.1572	-6.2755E+03	-8.4443E+00	6.2600E-06	2	278.68	562.16
13	C7H5CL3	BENZOTRICHLORIDE	50.6272	-7.4190E+03	-4.6513E+00	1.7396E-18	6	268.40	737.00
14	C7H7CL	BENZYL CHLORIDE	49.8582	-7.1698E+03	-4.4836E+00	1.3858E-18	6	234.15	686.00
15	C12H10	BIPHENYL	122.1472	-1.2321E+04	-1.4955E+01	5.6056E-06	2	342.37	780.26
16	C2H4CL2O	BIS(CHLOROMETHYL)ETHER	56.1552	-6.3984E+03	-5.4972E+00	8.2034E-18	6	231.65	579.00
17	CHBR3	BROMOFORM	53.1752	-6.7653E+03	-5.0514E+00	2.9653E-18	6	281.20	696.00
18	C4H6	1,3-BUTADIENE	69.2092	-4.5800E+03	-8.2922E+00	1.1820E-05	2	164.25	425.37
19	C6H11ON	CAPROLACTAM	69.2792	-1.0469E+04	-6.8944E+00	1.2113E-18	6	342.36	806.00
20	CS2	CARBON DISULFIDE	57.9042	-4.7063E+03	-6.7794E+00	8.0195E-03	1	161.11	552.00
21	CCL4	CARBON TETRACHLORIDE	73.5462	-6.1281E+03	-8.5763E+00	6.8461E-06	2	250.33	556.35
22	C2H3CLO2	CHLOROACETIC ACID	98.2572	-1.0585E+04	-1.1348E+01	4.1435E-06	2	333.15	686.00
23	C8H7CLO	2-CHLOROACETOPHENONE	----	----	----	----	-	---	---
24	C6H5CL	CHLOROBENZENE	44.7492	-5.9408E+03	-3.9391E+00	1.1417E-06	2	227.95	632.35
25	CHCL3	CHLOROFORM	130.3672	-7.4746E+03	-1.8700E+01	2.1909E-02	1	209.63	536.40
26	C4H5CL	CHLOROPRENE	42.9902	-4.7595E+03	-3.7996E+00	1.1726E-17	6	143.15	525.00
27	C7H8O	M-CRESOL	242.9872	-1.6060E+04	-3.5083E+01	2.8800E-02	1	285.39	705.85
28		CRESOLS/CRESYLIC ACID(ISOMERS & MIXTURES)	----	----	----	----	-	---	---
29	C7H8O	O-CRESOL	205.9872	-1.3928E+04	-2.9483E+01	2.5182E-02	1	304.19	697.55
30	C7H8O	P-CRESOL	282.9872	-1.7540E+04	-4.1637E+01	3.6171E-02	1	307.93	704.65
31	C9H12	CUMENE	82.7612	-8.3340E+03	-9.3567E+00	1.3600E-17	6	177.14	631.15
32	C6H4CL2	1,4-DICHLOROBENZENE	83.4172	-8.4634E+03	-9.6308E+00	4.5833E-06	2	326.14	684.75
33	C4H8CL2O	DICHLOROETHYL ETHER	----	----	----	----	-	---	---
34	C3H4CL2	1,3-DICHLOROPROPENE*	44.1267	-5.3347E+03	-3.9572E+00	6.9674E-18	6	191.50	577.00
35	C4H11NO2	DIETHANOLAMINE	281.1172	-2.0360E+04	-4.0422E+01	3.2378E-02	1	301.15	542.04
36	C8H11N	N,N-DIMETYLANILINE	46.4592	-7.1600E+03	-4.0127E+00	8.1481E-07	2	275.60	687.15
37	C4H10O4S	DIETHYL SULFATE	86.4342	-9.2791E+03	-1.0340E+01	6.8675E-03	1	248.00	483.00
38	C14H20N	DIMETHYLBENZIDINE	----	----	----	----	-	---	---
39	C3H7N	DIMETHYL FORMAMIDE	110.7172	-9.8538E+03	-1.3393E+01	2.1867E-17	6	212.72	647.00
40	C2H8N2	1,1-DIMETHYLHYDRAZINE	----	----	----	----	-	---	---
41	C10H10O4	DIMETHYL PHTHALATE	66.1802	-1.0534E+04	-6.4298E+00	1.0804E-18	6	272.15	766.00
42	C2H6SO4	DIMETHYL SULFATE	78.1512	-8.8719E+03	-8.5921E+00	1.8941E-06	2	241.35	758.00
43	C6H3N2O4	2,4-DINITROPHENOL	----	----	----	----	-	---	---
44	C7H6N2O4	2,4-DINITROTOLUENE	26.7022	-6.9259E+03	-1.6468E+00	3.6725E-03	1	343.00	814.00
45	C4H8O2	1,4-DIOXANE	47.3782	-5.6777E+03	-4.3645E+00	1.9626E-06	2	284.95	587.00
46	C12H12N2	1,2-DIPHENYLHYDRAZINE	89.6402	-1.2785E+04	-9.5673E+00	1.6660E-18	6	404.15	573.00
47	C3H5CLO	EPICHLOROHYDRIN	57.0212	-6.6420E+03	-5.6252E+00	1.2280E-06	2	215.95	610.00
48	C5H8O2	ETHYL ACRYLATE	126.6672	-8.2672E+03	-1.7694E+01	1.8538E-02	1	201.95	553.00
49	C8H10	ETHYLBENZENE	83.3532	-7.6911E+03	-9.7970E+00	5.9310E-06	2	178.15	617.17
50	C2H5CL	ETHYL CHLORIDE	65.2662	-4.7867E+03	-7.5387E+00	9.3370E-06	2	134.80	460.35

TABLE D-1 (CONTINUED)

$\ln P = A + B/T + C \ln T + D T^E$ (P - mm Hg, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
51	C2H4BR2	ETHYLENE BROMIDE	38.8582	-5.5877E+03	-3.0891E+00	8.2664E-07	2	282.85	650.15
52	C2H4CL2	ETHYLENE DICHLORIDE	111.4972	-7.3230E+03	-1.5370E+01	1.6794E-02	1	237.49	561.00
53	C2H6O2	ETHYLENE GLYCOL	189.7472	-1.4615E+04	-2.5433E+01	2.0140E-05	2	260.15	645.00
54	C2H4O	ETHYLENE OXIDE	91.9272	-5.4330E+03	-1.2517E+01	1.6080E-02	1	160.71	469.15
55	C2H4CL2	ETHYLIDENE DICHLORIDE	76.8602	-6.0103E+03	-9.1336E+00	8.5940E-06	2	176.19	523.00
56	CH2O	FORMALDEHYDE	96.6172	-4.9172E+03	-1.3765E+01	2.2031E-02	1	181.15	408.00
57	C4H10O2	ETHYLENE GLYCOL DIMETHYL ETHER	80.1902	-6.3722E+03	-1.0083E+01	9.9499E-03	1	215.15	536.15
58	C4H10O2	ETHYLENE GLYCOL MONOETHYL ETHER	266.7972	-1.3845E+04	-4.0900E+01	4.8096E-02	1	183.00	569.00
59	C8H16O4	DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE	105.8972	-9.9058E+03	-1.3729E+01	1.2203E-02	1	248.15	660.00
60	C6H12O3	ETHYLENE GLYCOL MONOETHYL ETHER ACETATE	79.6572	-8.6783E+03	-8.7244E+00	1.0459E-17	6	211.45	597.00
61	C6H14O3	DIETHYLENE GLYCOL MONOETHYL ETHER	250.9672	-1.7164E+04	-3.4699E+01	2.5107E-05	2	250.00	632.00
62	C5H10O3	ETHYLENE GLYCOL MONOMETHYL ETHER ACETATE*	80.0053	-8.6783E+03	-8.7244E+00	1.0459E-17	6	211.45	597.00
63	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL ETHER	173.6772	-1.5712E+04	-2.1908E+01	2.8569E-17	6	205.15	654.00
64	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	78.2492	-8.2848E+03	-8.6687E+00	1.9629E-17	6	203.15	432.91
65	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER	353.1672	-1.6390E+04	-5.5450E+01	6.6861E-02	1	225.00	564.00
66	C6H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	65.3342	-7.7712E+03	-6.6964E+00	2.2398E-17	6	183.15	582.00
67	C8H10O2	ETHYLENE GLYCOL MONOPHENYL ETHER*	108.8519	-1.0705E+04	-1.3140E+01	2.9781E-17	6	203.15	600.00
68	C5H12O2	DIETHYLENE GLYCOL MONOMETHYL ETHER	428.7372	-2.1730E+04	-6.6416E+01	6.9903E-02	1	250.00	630.00
69	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	71.5962	-8.5825E+03	-7.6847E+00	3.6009E-06	2	228.85	624.00
70	C6H14O2	ETHYLENE GLYCOL MONOBUTYL ETHER	110.6072	-1.0705E+04	-1.3140E+01	2.9781E-17	6	203.15	600.00
71	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	98.8572	-1.1633E+04	-1.1067E+01	6.2208E-18	6	229.35	651.00
72	C8H15O3	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE*	78.7842	-8.6783E+03	-8.7244E+00	1.0459E-17	6	211.45	597.00
73	C6CL6	HEXACHLOROBENZENE	158.3372	-1.8324E+04	-1.8899E+01	2.3902E-18	6	501.70	825.00
74	C4CL6	HEXACHLOROBUTADIENE	81.9512	-9.5280E+03	-9.0606E+00	1.3588E-06	2	252.15	741.00
75	C2CL6	HEXACHLOROETHANE	430.2172	-2.7220E+04	-6.0495E+01	3.0865E-05	2	459.95	512.25
76	C6H14	HEXANE	160.5772	-8.3533E+03	-2.3927E+01	2.9469E-02	1	177.84	507.43
77	C6H6O2	HYDROQUINONE	105.9772	-1.2856E+04	-1.2677E+01	6.9120E-03	1	444.65	822.00
78	C9H14O	ISOPHORONE	78.1382	-8.1126E+03	-9.5117E+00	8.1784E-03	1	265.05	715.00
79	C4H2O3	MALEIC ANHYDRIDE	63.9872	-7.7226E+03	-7.2087E+00	7.0169E-03	1	326.00	710.00
80	CH4O	METHANOL	105.0372	-7.4713E+03	-1.3988E+01	1.5281E-02	1	175.47	512.58
81	CH3BR	METHYL BROMIDE	67.6932	-4.6986E+03	-7.9966E+00	1.1553E-05	2	179.47	467.00
82	CH3CL	METHYL CHLORIDE	59.2372	-4.0301E+03	-6.7151E+00	1.0210E-05	2	175.43	416.25
83	C2H3CL3	METHYL CHLOROFORM	84.1522	-6.5442E+03	-1.0205E+01	8.5368E-06	2	242.75	545.00
84	C4H8O	METHYL ETHYL KETONE	109.8472	-7.1300E+03	-1.5184E+01	1.7234E-02	1	186.48	535.50
85	CH6N2	METHYL HYDRAZINE	----	----	----	----	-	---	---
86	C6H12O	METHYL ISOBUTYL KETONE	147.8072	-1.0034E+04	-1.9766E+01	1.6353E-05	2	189.15	571.40
87	C2H3NO	METHYL ISOCYANATE	41.7632	-4.4556E+03	-3.6339E+00	1.5024E-17	6	256.15	505.00
88	C5H8O2	METHYL METHACRYLATE	246.1372	-1.2144E+04	-3.7654E+01	4.2873E-02	1	224.95	564.00
89	C5H12O	METHYL TERT-BUTYL ETHER	50.9812	-5.1301E+03	-4.9617E+00	1.9765E-17	6	164.55	497.10
90	CH2CL2	METHYLENE CHLORIDE	74.9742	-5.7947E+03	-8.8015E+00	7.6432E-06	2	178.01	510.00
91	C15H10N2O2	METHYLENE DIPHENYL DIISOCYANATE	78.9502	-1.3604E+04	-7.8429E+00	6.0025E-18	6	311.20	609.00
92	C13H14N2	4,4-METHYLENEDIANILINE	----	----	----	----	-	---	---
93	C10H8	NAPHTHALENE	80.3972	-9.0622E+03	-9.0648E+00	3.5805E-06	2	353.43	748.35
94	C6H5NO2	NITROBENZENE	85.5522	-9.7448E+03	-9.5228E+00	7.5659E-18	6	---	---
95	C6H5NO3	2-NITROPHENOL	----	----	----	----	-	---	---
96	C3H7NO2	2-NITROPROPANE	51.5512	-6.2903E+03	-4.8462E+00	9.2273E-18	6	181.83	594.00
97	C6H6O	PHENOL	54.1872	-8.0500E+03	-4.8990E+00	2.800E-04	1	314.06	694.25
98	C6H8N2	P-PHENYLENEDIAMINE	79.0322	-1.1341E+04	-8.1769E+00	1.5761E-18	6	413.00	796.00
99	COCL2	PHOSGENE	107.4272	-5.6774E+03	-1.5351E+01	2.1250E-02	1	145.37	455.00
100	C8H4O3	PHTHALIC ANHYDRIDE	70.5352	-8.9302E+03	-7.8671E+00	5.9603E-06	2	404.15	791.00

TABLE D-1 (CONTINUED)

NO	FORMULA	NAME	ln P = A + B/T + C ln T + D T^E (P - mm Hg, T - K) A	B	C	D	E	TMIN	TMAX
101	C3H4O2	BETA-PROPIOLACTONE	59.6992	-7.8204E+03	-5.7808E+00	3.0689E-18	6	239.75	685.00
102	C3H6O	PROPIONALDEHYDE	60.2442	-5.3095E+03	-6.5289E+00	5.8611E-06	2	193.15	496.00
103	C3H6CL2	PROPYLENE DICHLORIDE	49.2312	-5.6774E+03	-4.6063E+00	9.0212E-18	6	172.71	572.00
104	C3H6O	PROPYLENE OXIDE	88.7372	-6.0580E+03	-1.1104E+01	1.2670E-05	2	161.22	482.25
105	C6H4O2	QUINONE	----	----	----	----	-	---	---
106	C8H8	STYRENE	128.6272	-9.2655E+03	-1.7609E+01	1.5391E-02	1	242.54	648.00
107	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	129.4872	-1.0273E+04	-1.6556E+01	9.3081E-06	2	229.35	645.00
108	C2CL4	TETRACHLOROETHYLENE	53.8712	-6.1912E+03	-5.3312E+00	2.1269E-06	2	250.80	620.00
109	C7H8	TOLUENE	78.4662	-6.9950E+03	-9.1635E+00	6.2250E-06	2	178.18	591.79
110	C7H10N2	2,4-TOLUENE DIAMINE	100.9772	-1.2648E+04	-1.1472E+01	2.9007E-06	2	371.25	804.00
111	C9H6N2O2	2,4-TOLUENE DIISOCYANATE	95.0812	-1.1659E+04	-1.0583E+01	4.1543E-18	6	287.04	737.00
112	C7H9N	O-TOLUIDINE	222.3572	-1.4424E+04	-3.2263E+01	2.8462E-02	1	249.47	694.15
113	C6H3CL3	1,2,4-TRICHLOROBENZENE	35.9082	-6.6591E+03	-2.5549E+00	4.6936E-04	1	290.15	725.00
114	C2H3CL3	1,1,2-TRICHLOROETHANE	57.7592	-6.3017E+03	-5.9182E+00	2.7241E-06	2	236.50	302.00
115	C2HCL3	TRICHLROETHYLENE	54.5102	-5.4716E+03	-5.8275E+00	4.5098E-03	1	188.40	571.15
116	C6H3CL3O	2,4,5-TRICHLOROPHENOL	----	----	----	----	-	---	---
117	C6H15N	TRIETHYLAMINE	51.6572	-5.6819E+03	-4.9815E+00	1.2363E-17	6	158.45	535.15
118	C8H18	2,2,4-TRIMETHYLPENTANE	115.9172	-7.5500E+03	-1.6111E+01	1.7099E-02	1	165.78	543.96
119	C4H6O2	VINYL ACETATE	43.0492	-5.2462E+03	-3.6360E+00	4.5798E-18	6	180.35	524.00
120	C2H3CL	VINYL CHLORIDE	121.9572	-5.7601E+03	-1.7914E+01	2.4917E-02	1	119.36	431.55
121	C2H2CL2	VINYLIDENE CHLORIDE	67.7482	-5.4481E+03	-7.5697E+00	7.0922E-17	6	10.59	482.00
122		XYLENES (ISOMERS & MIXTURES)	----	----	----	----	-	---	---
123	C8H10	M-XYLENE	79.8542	-7.5941E+03	-9.2570E+00	5.5500E-06	2	225.30	617.05
124	C8H10	O-XYLENE	85.7512	-7.9608E+03	-1.0126E+01	6.0150E-06	2	247.98	630.37
125	C8H10	P-XYLENE	138.2772	-9.2470E+03	-1.9441E+01	1.9084E-02	1	286.41	616.26

• - Estimated values for coefficients in vapor pressure equation.
ln = natural logarithm
Primary data source: Daubert, T. E. and R. P. Danner, DATA COMPILATION OF PROPERTIES OF PURE COMPOUNDS, Parts 1,2,3 and 4, Supplements 1 and 2, DIPPR Project, AIChE, New York, NY (1985-1992).

TABLE D-2 VAPOR PRESSURE - ANTOINE EQUATION

NO	FORMULA	NAME	log P = A - B/(T+C) (P - mm Hg, T - C) A	B	C	TMIN	TMAX
11	C7H9NO	O-ANISIDINE	8.30799	2475.780	237.134	61	218
33	C4H8CL2O	DICHLOROETHYL ETHER	7.69239	1990.755	235.347	23	178
40	C2H8N2	1,1-DIMETHYLHYDRAZINE	7.58826	1388.510	232.537	-35	20
85	CH6N2	METHYL HYDRAZINE	6.84297	1115.190	191.648	2	25
116	C6H3CL3O	2,4,5-TRICHLOROPHENOL	7.82316	2420.564	237.476	72	252

log = logarithm to base 10

Primary data source: Ohe, S., COMPUTER AIDED DATA BOOK OF VAPOR PRESSURE, Data Book Publishing Company, Tokyo, Japan (1976).

APPENDIX E

WATER SOLUBILITY

No	Formula	Name	Solubility in Water @ 25 C ppm(wt)	Source
4	C8H8O	ACETOPHENONE	6842.00	Selected
			6842.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
5	C3H4O	ACROLEIN	245700.00	Selected
			245700.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
8	C3H3N	ACRYLONITRILE	77240.00	Selected
			77240.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			74900.00	Kirk, R. E. and D. F. Othmer, eds., ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY, 3rd ed., Vol. 11, John Wiley and Sons, Inc., New York, NY (1980).
9	C3H5CL	ALLYL CHLORIDE	4000.00	Selected
			4000.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
10	C6H7N	ANILINE	34160.00	Selected
			34160.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
12	C6H6	BENZENE	1755.17	Selected
			1755.17	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			1780.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			1755.00	McDevit, W. F. and F. A. Long, J. Am. Chem. Soc., 74, 1773 (1952).
			1769.00	Mackay, D., M. Aquan-Yuen and W. Y. Shiu, J. Chem. Eng. Data, 24, 30 (1979).
			1790.00	Bohon, R. L. and W. F. Claussen, J. Am. Chem. Soc., 73, 1571 (1951).
			1779.50	Mackay, D. and W. Y. Shiu, Can. J. Chem.

				Eng., 53, 239 (1975).
			1740.00	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			1869.00	Klevens, H. B., J. Phys. Colloid Chem., 54, 283 (1950).
15	C12H10	BIPHENYL	7.00	Selected
			7.00	Mackay, D. and W. Y. Shiu, J. Chem. Eng. Data, 22, 399 (1977).
			7.45	Eganhouse, R. P. and J. A. Calder, Geochim. et Cosmochim. Acta, 40, 555 (1976).
			7.08	Wauchope, R. D. and F. W. Getzen, J. Phys. Chem. Data, 17, 38 (1972).
			5.94	Andrews, L. J. and R. M. Keefer, J. Am. Chem. Soc., 71, 3644 (1949).
			3.87	Sahyunm, M. R., Nature, 209, 613 (1966).
17	CHBR3	BROMOFORM	3090.00	Selected
			3090.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
18	C4H6	1,3-BUTADIENE	735.00	Selected
			735.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
20	CS2	CARBON DISULFIDE	1879.00	Selected
			1879.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
21	CCL4	CARBON TETRACHLORIDE	785.70	Selected
			785.70	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			800.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
24	C6H5CL	CHLOROBENZENE	503.00	Selected
			471.70	Mackay, D., R. J. Sutherland and W. Y. Shiu, Environ. Sci. Technol., 8, 333 (1979).
			500.00	Andrews, L. J. and R. M. Keefer, J. Am. Chem. Soc., 72, 3113 (1950).
			490.00	Gross, P. M. and J. H. Taylor, J. Am. Chem. Soc., 53, 1744 (1931).
			503.00	Yalkowsky, S. H., R. J. Orr and S. C. Valvani, I & EC Fundam., 18, 351 (1979)
25	CHCL3	CHLOROFORM	7842.70	Selected
			7842.70	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part

				1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			7800.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
27	C7H8O	M-CRESOL	22625.00	Selected
			22625.00	Stephen, H. and T. Stephen, SOLUBILITIES OF INORGANIC AND ORGANIC COMPOUNDS, Vol. 1, Part 1, Macmillan Company, New York, NY (1963).
29	C7H8O	O-CRESOL	26075.00	Selected
			26075.00	Stephen, H. and T. Stephen, SOLUBILITIES OF INORGANIC AND ORGANIC COMPOUNDS, Vol. 1, Part 1, Macmillan Company, New York, NY (1963).
30	C7H8O	P-CRESOL	20200.00	Selected
			20200.00	Stephen, H. and T. Stephen, SOLUBILITIES OF INORGANIC AND ORGANIC COMPOUNDS, Vol. 1, Part 1, Macmillan Company, New York, NY (1963).
31	C9H12	CUMENE	50.00	Selected
			50.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			48.30	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			65.30	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
32	C6H4CL2	1,4-DICHLOROBENZENE	83.10	Selected
			83.10	Mackay, D. and W. Y. Shiu, unpublished results (1981)
			87.20	Wauchope, R. D. and F. W. Getzen, J. Phys. Chem. Data, 17, 38 (1972).
			79.00	Seidell. A., SOLUBILITIES OF ORGANIC COMPOUNDS, Vol. III, 3rd ed., Van Nostrand Co., New York, NY (1941).
			90.60	Yalowsky, S. H., R. J. Orr and S. C. Valvani, I & EC Fundam., 18, 351 (1979)
34	C3H4CL2	1,3-DICHLOROPROPENE	2730.00	Selected
			2730.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
49	C8H10	ETHYLBENZENE	165.13	Selected
			165.13	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			152.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			177.00	Polak, J. and B. C. Y. Lu, Can. J. Chem. 51, 4018 (1973).
			131.00	Price, L. C., Bull. Am. Assoc. Petrol.

				Geologists, 60(2), 213 (1976).
			208.00	Bohon, R. L. and W. F. Claussen, J. Am. Chem. Soc., 73, 1571 (1951).
			161.00	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
			175.00	Klevens, H. B., J. Phys. Colloid Chem., 54, 283 (1950).
50	C2H5CL	ETHYL CHLORIDE	5700.00	Selected
			5700.00 @ 20 C	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
51	C2H4BR2	ETHYLENE BROMIDE	4118.00	Selected
			4118.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
52	C2H4CL2	ETHYLENE DICHLORIDE	8679.00	Selected
			8679.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			10600.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
55	C2H4CL2	ETHYLIDENE DICHLORIDE	5032.00	Selected
			5032.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			5030.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
60	C6H12O3	ETHYLENE GLYCOL MONOETHYL ETHER ACETATE	229000.00	Selected
			229000.00	Kirk, R. E. and D. F. Othmer, eds., ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY, 3rd ed., Vol. 11, John Wiley and Sons, Inc., New York, NY (1980).
67	C8H10O2	ETHYLENE GLYCOL MONOPHENYL ETHER	27000.00	Selected
			27000.00	Kirk, R. E. and D. F. Othmer, eds., ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY, 3rd ed., Vol. 11, John Wiley and Sons, Inc., New York, NY (1980).
72	C8H15O3	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE	15000.00	Selected
			15000.00	Kirk, R. E. and D. F. Othmer, eds., ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY, 3rd ed., Vol. 11, John Wiley and Sons, Inc., New York, NY (1980).
73	C6CL6	HEXACHLOROBENZENE	0.005	Selected
			0.005	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
74	C4CL6	HEXACHLOROBUTADIENE	3.23	Selected

			3.23	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
75	C2CL6	HEXACHLOROETHANE	8.00	Selected
			8.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
76	C6H14	HEXANE	9.47	Selected
			9.5000	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			9.4700	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			9.5200	Baker, E. G., FUNDAMENTAL ASPECTS OF PETROLEUM GEOCHEMISTRY, Nagy, B. and U. Colombo, eds., Chapter 7, 299, Elsevier Publishing Co., New York, NY (1967).
			12.3000	Mackay, D., M. Aquan-Yuen and W. Y. Shiu, J. Chem. Eng. Data, 24, 30 (1979).
			12.4000	Polak, J. and B. C. Y. Lu, Can. J. Chem., 51, 4018 (1973).
81	CH3BR	METHYL BROMIDE	13410.00	Selected
			13410.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
82	CH3CL	METHYL CHLORIDE	5900.00	Selected
			5900.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
83	C2H3CL3	METHYL CHLOROFORM	700.00	Selected
			700.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
84	C4H8O	METHYL ETHYL KETONE	248600.00	Selected
			248600.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
89	C5H12O	METHYL TERT-BUTYL ETHER	52100.00	Selected
			52100.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
90	CH2CL2	METHYLENE CHLORIDE	19380.00	Selected
			19380.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			19400.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
93	C10H8	NAPHTHALENE	31.70	Selected
			34.40	Bohon, R. L. and W. F. Claussen, J. Am.

				Chem. Soc., 73, 1571 (1951).
			31.20	Wauchope, R. D. and F. W. Getzen, J. Phys. Chem. Data, 17, 38 (1972).
			31.70	Mackay, D. and W. Y. Shiu, J. Chem. Eng. Data, 22, 399 (1977).
94	C6H5NO2	NITROBENZENE	1936.00	Selected
			1936.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
96	C3H7NO2	2-NITROPROPANE	17000.00	Selected
			17000.00	Lange, N. A., ed., HANDBOOK OF CHEMISTRY, 10th ed. (revised), McGraw-Hill, New York, NY (1969).
97	C6H6O	PHENOL	80190.00	Selected
			80190.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
102	C3H6O	PROPIONALDEHYDE	404720.00	Selected
			404720.00	Macedo, E. A. and P. Rasmussen, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Supplement 1, Vol. V, Part 4, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1987).
103	C3H6CL2	PROPYLENE DICHLORIDE	2750.00	Selected
			2750.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			2800.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
106	C8H8	STYRENE	321.60	Selected
			321.60	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
107	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	2900.00	Selected
			2900.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			2900.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
108	C2CL4	TETRACHLOROETHYLENE	150.00	Selected
			150.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
109	C7H8	TOLUENE	542.37	Selected
			542.37	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part

				1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			515.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			517.00	Mackay, D., W. Y. Shiu and A. W. Wolkoff, ASTM 573, 251 (1975).
			544.00	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			534.30	Schwarz, F. P. and S. P. Wasik, J. Chem. Eng. Data, 22, 270 (1977).
			500.00	Klevens, H. B., J. Phys. Colloid Chem., 54, 283 (1950).
			519.50	Mackay, D. and W. Y. Shiu, Can. J. Chem. Eng., 53, 239 (1975).
			627.00	Bohon, R. L. and W. F. Claussen, J. Am. Chem. Soc., 73, 1571 (1951).
114	C2H3CL3	1,1,2-TRICHLOROETHANE	4393.00	Selected
			4393.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			4380.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
115	C2HCL3	TRICHLROETHYLENE	1100.00	Selected
			1100.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
117	C6H15N	TRIETHYLAMINE	72930.00	Selected
			72930.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
118	C8H18	2,2,4-TRIMETHYLPENTANE	2.221	Selected
			2.221	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			2.4400	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			2.0500	Polak, J. and B. C. Y. Lu, Can. J. Chem., 51, 4018 (1973).
119	C4H6O2	VINYL ACETATE	25530.00	Selected
			25530.00	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
120	C2H3CL	VINYL CHLORIDE	2763.00	Selected
			2763.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
121	C2H2CL2	VINYLIDENE CHLORIDE	3345.00	Selected

			3345.00	Horvath, A. L., HALOGENATED HYDROCARBONS, Marcel Dekker, Inc., New York, NY (1982).
123	C8H10	M-XYLENE	173.97	Selected
			173.97	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			162.00	Polak, J. and B. C. Y. Lu, Can. J. Chem. 51, 4018 (1973).
			196.00	Bohon, R. L. and W. F. Claussen, J. Am. Chem. Soc., 73, 1571 (1951).
			173.00	Andrews, L. J. and R. M. Keefer, J. Am. Chem. Soc., 71, 3644 (1949).
			146.00	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
			134.00	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
124	C8H10	O-XYLENE	220.83	Selected
			220.83	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			175.00	McAuliffe, C., J. Phy. Chem., 70, 1267 (1966).
			170.00	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
			167.00	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			204.00	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
			213.00	Polak, J. and B. C. Y. Lu, Can. J. Chem. 51, 4018 (1973).
125	C8H10	P-XYLENE	201.68	Selected
			201.68	Sørensen, J. M. and W. Arlt, LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION, Vol. V, part 1, Dechema Chemistry Data Series, 6000 Frankfurt/Main, Germany (1979).
			185.00	Polak, J. and B. C. Y. Lu, Can. J. Chem. 51, 4018 (1973).
			198.00	Bohon, R. L. and W. F. Claussen, J. Am. Chem. Soc., 73, 1571 (1951).
			157.00	Price, L. C., Bull. Am. Assoc. Petrol. Geologists, 60(2), 213 (1976).
			156.00	Sutton, C. and J. A. Calder, J. Chem. Eng. Data, 20, 320 (1975).
			200.00	Andrews, L. J. and R. M. Keefer, J. Am. Chem. Soc., 71, 3644 (1949).

ppm(wt) = parts per million (weight)

APPENDIX F

ACTIVITY COEFFICIENT AT INFINITE DILUTION

No	Formula	Name	Activity Coeff. at Infinite Dilution γ^{∞}	Source
1	C2H4O	ACETALDEHYDE	5.51	Selected
			5.51	Byk, S. Sh., I. I. Serebrennaya and P. R. Scherbakova, Khim. Prom., 7, 507 (1963).
			5.83	INTERNATIONAL CRITICAL TABLES, McGraw-Hill, New York, NY (1928).
			3.30	D'Avila, S. G. and R. S. F. Silva, J. Chem. Eng. Data, 15, 421 (1970).
2	C2H5ON	ACETAMIDE	1.54	Estimated UNIFAC
3	C2H3N	ACETONITRILE	9.48	Selected
			9.81	Blackford, D. S. and R. York, J. Chem. Eng. Data, 10, 313 (1965).
			9.48	Maslan, F. D. and E. A. Stoddard, J. Phys. Chem., 60, 1146 (1956).
			9.24	Vierk, A. L., Z. Anorg. Chem., 261, 283 (1950).
6	C3H5NO	ACRYLAMIDE	1.54	Estimated UNIFAC
7	C3H4O2	ACRYLIC ACID	2.12	Selected
			2.12	Linek, J. and I. Wichterle, Collect. Czech. Chem. Commun., 39, 3395 (1974).
			3.62	Frolov, A. F., M. A. Loginova, B. F. Ustavshchikov and others, Zh. Fiz. Khim. 41, 2088 (1967).
11	C7H9NO	O-ANISIDINE	96.20	Estimated
13	C7H5CL3	BENZOTRICHLORIDE	88265.24	Estimated
14	C7H7CL	BENZYL CHLORIDE	10328.89	Estimated
16	C2H4CL2O	BIS(CHLOROMETHYL)ETHER	129.93	Estimated
19	C6H11ON	CAPROLACTAM	20.73	Estimated
22	C2H3CLO2	CHLOROACETIC ACID	12.77	Estimated
23	C8H7CLO	2-CHLOROACETOPHENONE	4699.21	Estimated
26	C4H5CL	CHLOROPRENE	179.67	Estimated
33	C4H8CL2O	DICHLOROETHYL ETHER	522.71	Estimated
35	C4H11NO2	DIETHANOLAMINE	1.35	Estimated
36	C8H11N	N,N-DIMETYLANILINE	827.16	Estimated

38	C14H20N	DIMETHYLBENZIDINE	13560.11	Estimated
39	C3H7NO	DIMETHYL FORMAMIDE	2.04	Selected
			1.88	Susarev, M. P., Zh. Prikl. Khim., 34, 412 (1961).
			2.04	Di Cave, S. and A. R. Giona, Ric. Sci. Rend., 34, A4, 645 (1964).
40	C2H8N2	1,1-DIMETHYLHYDRAZINE	0.44	Selected
			0.44	Carleton, L. T., Ind. Eng. Chem. Chem. Eng. Data Series, 1, 21 (1956).
41	C10H10O4	DIMETHYL PHTHALATE	13560.11	Estimated
43	C6H3N2O4	2,4-DINITROPHENOL	235.44	Estimated
44	C7H6N2O4	2,4-DINITROTOLUENE	16152.54	Estimated
45	C4H8O2	1,4-DIOXANE	6.10	Selected
			6.10	Kortuem, G., D. Moegling and F. Woerner, Chem. Ing. Tech., 22, 453 (1950).
			8.25	Smith, E. R. and M. J. Wojciechowski, J. Res. Nat. Bur. Stand. Sect. A, 18, 461 (1937).
47	C3H5ClO	EPICHLOROHYDRIN	20.43	Estimated
48	C5H8O2	ETHYL ACRYLATE	111.41	Estimated
53	C2H6O2	ETHYLENE GLYCOL	0.87	Selected
			0.87	Villamanan, M. A., C. Gonzalez and H. C. Van Ness, J. Chem. Eng. Data, 29, 427 (1984).
			0.90	Villa Rivera, J. E., Thesis, Paris, 1983.
54	C2H4O	ETHYLENE OXIDE	7.64	Selected
			5.74	McCormack, K. E. and J. H. B. Chenier, Ind. Eng. Chem., 47, 1454 (1955).
			7.64	Gillespie, P. C., J. R. Cunningham and G. M. Wilson, AIChE Symposium Series No. 244, 81, 26 (1985).
56	CH2O	FORMALDEHYDE	1.50	Estimated
57	C4H10O2	ETHYLENE GLYCOL DIMETHYL ETHER	19.38	Selected
			19.38	Hunsmann, W. and K. H. Simmrock, Chem. Ing. Tech., 38, 1053 (1966).
58	C4H10O2	ETHYLENE GLYCOL MONOETHYL ETHER	6.87	Selected
			6.87	Boublik, T. and K. Kuchynka, Chem. Listy, 50, 1181 (1956).
			5.61	Dominik, W. and J. Wojciechowska, Przem. Chem., 23, 61 (1939).
59	C8H16O4	DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE	184.13	Estimated
61	C6H14O3	DIETHYLENE GLYCOL MONOETHYL ETHER	16.14	Estimated
62	C5H10O3	ETHYLENE GLYCOL MONOMETHYL ETHER ACETATE	27.97	Estimated

63	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL ETHER	43.43	Estimated
64	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	21.51	Estimated
65	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER	4.40	Estimated
66	C6H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	11.62	Estimated
68	C5H12O2	DIETHYLENE GLYCOL MONOMETHYL ETHER	9.54	Estimated
69	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	173.80	Estimated
70	C6H14O2	ETHYLENE GLYCOL MONOBUTYL ETHER	19.84	Selected
			14.82	Newman, M., C. B. Hayworth and R. E. Treybal, Ind. Eng. Chem., 41, 2039 (1949).
			22.23	Schneider, G. and G. Wilhelm, Z. Phys. Chem. (Frankfurt), 20, 219 (1959).
			19.84	Scatchard, G. and G. M. Wilson, J. Am. Chem. Soc., 86, 133 (1964).
71	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	48.92	Estimated
77	C8H6O2	HYDROQUINONE	19.07	Estimated
78	C9H14O	ISOPHORONE	3818.97	Estimated
79	C4H2O3	MALEIC ANHYDRIDE	22.62	Estimated
80	CH4O	METHANOL	2.15	Selected
			2.15	Green, S. I. and R. E. Venner, Ind. Eng. Chem., 47, 103 (1955).
			2.24	Dunlop, J. G., M. S. Thesis, Brooklyn Polytechn. Inst., 1948.
85	CH6N2	METHYL HYDRAZINE	0.38	Estimated
88	C5H8O2	METHYL METHACRYLATE	93.17	Estimated
92	C13H14N2	4,4-METHYLENEDIANILINE	3307.87	Estimated
95	C6H5NO3	2-NITROPHENOL	76.56	Estimated
98	C6H8N2	P-PHENYLENEDIAMINE	14.23	Estimated
100	C8H4O3	PHTHALIC ANHYDRIDE	243.68	Estimated
101	C3H4O2	BETA-PROPIOLACTONE	2.84	Estimated
104	C3H6O	PROPYLENE OXIDE	28.19	Selected
			28.19	Wickert, J. N., W. S. Tamplin and R. L. Shank, Chem. Eng. Progr. Symp. Ser. 48, 92 (1952).
105	C6H4O2	QUINONE	53.58	Estimated
110	C7H10N2	2,4-TOLUENE DIAMINE	39.41	Estimated
112	C7H9N	O-TOLUIDINE	308.64	Estimated
113	C6H3CL3	1,2,4-TRICHLOROBENZENE	13249.06	Estimated
116	C6H3CL3O	2,4,5-TRICHLOROPHENOL	670.22	Estimated

Estimated - UNIFAC (group contribution method)