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Improved Prediction of Octanol-Water Partition Coefficients from Liquid-Solute Water Solubilities and Molar Volumes

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Summary of the Information

Tables showing selected water solubilities (log S_w), molar volumes (log $\overline{V}$), perfect-solution partition coefficients (log K^{o}_{sw}), and predicted and selected octanol-water partition coefficients (log K_{ow}) for compounds of various chemical classes at 25 ºC are presented.

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Table 1S. Predicted log K_{ow} values for aliphatic hydrocarbons (ALHCs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)	log $\overline{V}$ (L/mol)[a]	S_w^* (mg//L)	Ref	$\Delta\overline{H}_f$ (cal/mol)	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
n-Pentane	72.2	L[c]	-0.935	38.5	*2*	NA[d]	1	-3.27	4.21	3.56	3.62	*3*	0.06
n-Hexane	86.2	L	-0.881	9.50	*2*	NA	1	-3.96	4.84	4.11	4.11	*3*	0.00
n-Heptane	100.2	L	-0.832	2.93	*2*	NA	1	-4.53	5.37	4.57	4.66	*3*	0.09
n-Octane	114.2	L	-0.787	0.66	*2*	NA	1	-5.24	6.02	5.15	5.18	*3*	0.03
Cyclopentane	70.1	L	-1.026	156	*2*	NA	1	-2.65	3.68	3.10	3.00	*4*	-0.10
Cyclohexane	84.2	L	-0.963	55.8	*5*	NA	1	-3.18	4.15	3.51	3.44	*4*	-0.07
1-Hexene	84.2	L	-0.900	69.7	*3*	NA	1	-3.08	3.98	3.36	3.39	*3*	0.03
1-Heptene	98.2	L	-0.849	18.2	*3*	NA	1	-3.73	4.58	3.88	3.99	*3*	0.11
1-Octene	112.2	L	-0.802	2.70	*6*	NA	1	-4.62	5.42	4.62	4.57	*3*	-0.05
1-Nonene	126.2	L	-0.759	1.12	*3*	NA	1	-5.05	5.81	4.96	5.15	*3*	0.19
Cyclohexene	82.1	L	-0.992	213	*6*	NA	1	-2.59	3.58	3.01	2.86	*4*	-0.15
Cycloheptatriene	92.1	L	-0.984	620	*6*	NA	1	-2.17	3.16	2.64	2.63	*7*	-0.01
1-Pentyne	68.1	L	-0.935	1570	*6*	NA	1	-1.64	2.64	2.18	2.12	*3*	-0.06
1-Hexyne	82.2	L	-0.937	360	*6*	NA	1	-2.36	3.30	2.75	2.73	*3*	-0.02

[a] Molar volumes ($\overline{V}$) are obtained from liquid densities cited in Mackay et al. (*1*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC. [d] NA = not applicable for liquids.

Table 2S. Predicted log K_{ow} values for halogenated aliphatic hydrocarbons (HALHCs) at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)	log $\overline{V}$ (L/mol)[a]	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Dichloromethane	84.9	L[c]	-1.193	19400	*8*	NA[d]	1	-0.641	1.83	1.49	1.51	*9*	0.02
Chloroform	119.4	L	-1.093	7230	*10*	NA	1	-1.22	2.31	1.90	1.90	*10*	0.00
Carbon tetrachloride	153.8	L	-1.014	800	*8*	NA	1	-2.28	3.30	2.77	2.73	*10*	-0.04
1,2-Dichloroethane	99.0	L	-1.104	8700	*8*	NA	1	-1.06	2.16	1.77	1.76	*11*	-0.01
1,1,1-Trichloroethane	133.4	L	-0.999	1334	*12*	NA	1	-2.00	3.00	2.50	2.47	*12*	-0.03
1,1,2,2-Tetrachloroethane	167.9	L	-0.978	2970	*10*	NA	1	-1.75	2.73	2.26	2.39	*10*	0.13
Pentachloroethane	202.3	L	-0.918	500	*13*	NA	1	-2.61	3.52	2.95	2.89	*12*	-0.06
Trichloroethylene	132.0	L	-1.045	1366	*14*	NA	1	-1.98	3.03	2.53	2.53	*14*	0.00
Tetrachloroethylene	165.8	L	-0.991	200	*15*	NA	1	-2.92	3.91	3.30	3.38	*15*	0.08
Bromodichloromethane	163.8	L	-1.080	4700	*16*	NA	1	-1.54	2.62	2.18	2.10	*9*	-0.08
Ethyliodide	156.0	L	-1.093	4060	*17*	NA	1	-1.58	2.68	2.23	2.00	*18*	-0.23
1-Bromo-3-chloropropane	157.4	L	-1.005	2340	*14*	NA	1	-1.83	2.83	2.35	2.18	*14*	-0.17
1-Chlorobutane	92.6	L	-0.981	872	*14*	NA	1	-2.03	3.01	2.50	2.55	*14*	0.05
1-Bromobutane	137.0	L	-0.964	608	*19*	NA	1	-2.35	3.32	2.78	2.75	*20*	-0.03
1-Bromopentane	151.1	L	-0.904	127	*14*	NA	1	-3.08	3.98	3.35	3.37	*14*	0.02
1-Bromohexane	165.1	L	-0.831	25.8	*14*	NA	1	-3.81	4.64	3.93	3.80	*14*	-0.13
1-Chloroheptane	134.7	L	-0.816	13.6	*14*	NA	1	-4.00	4.81	4.08	4.15	*14*	0.07

1-Bromoheptane	179.1	L	-0.804	6.65	*14*	NA	1	-4.43	5.23	4.45	4.36	*14*	-0.09
1-Bromooctane	193.1	L	-0.763	1.67	*14*	NA	1	-5.06	5.83	4.97	4.89	*14*	-0.08
1-Iodoheptane	226.1	L	-0.785	3.50	*14*	NA	1	-4.81	5.60	4.77	4.70	*14*	-0.07
Hexachlorobutadiene	260.8	L	-0.810	2.55	*21*	NA	1	-5.01	5.82	4.97	4.90	*21*	-0.07
Hexachlorocyclopentadiene	272.8	L	-0.795	1.80	*22*	NA	1	-5.18	5.98	5.11	5.04	*22*	-0.07

[a] Molar volumes ($\overline{V}$) are obtained from liquid densities cited in Mackay et al. (*1*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 3S. Predicted log K_{ow} values for alkylbenzenes (ALBZs) at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Benzene	78.1	L[c]	-1.05	1780	*2*	NA[d]	1	-1.64	2.69	2.23	2.13	*18*	-0.10
Toluene	92.1	L	-0.974	517	*24*	NA	1	-2.25	3.22	2.69	2.69	*18*	0.00
Styrene	104.5	L	-0.936	300	*25*	NA	1	-2.54	3.48	2.91	2.95	*9*	0.04
Ethylbenzene	106.2	L	-0.912	159	*2*	NA	1	-2.82	3.74	3.14	3.15	*3*	0.01
1,2-Xylene	106.2	L	-0.918	175	*6*	NA	1	-2.78	3.70	3.11	3.13	*26*	0.02
1,3-Xylene	106.2	L	-0.920	160	*26*	NA	1	-2.82	3.74	3.15	3.20	*26*	0.05
1,4-Xylene	106.2	L	-0.909	157	*27*	NA	1	-2.83	3.74	3.14	3.18	*26*	0.04
1,2,3-Trimethylbenzene	120.2	L	-0.871	65.5	*14*	NA	1	-3.26	4.14	3.49	3.55	*14*	0.06
1,2,4-Trimethylbenzene	120.2	L	-0.863	57	*6*	NA	1	-3.32	4.19	3.53	3.63	*28*	0.10
1,3,5-Trimethylbenzene	120.2	L	-0.865	69.2	*29*	NA	1	-3.24	4.10	3.46	3.42	*30*	-0.04
1-Ethyl-2-methylbenzene	120.2	L	-0.865	74.6	*3*	NA	1	-3.21	4.07	3.43	3.53	*3*	0.10
n-Propylbenzene	120.2	L	-0.856	52.1	*26*	NA	1	-3.36	4.22	3.56	3.69	*26*	0.13
n-Butylbenzene	134.2	L	-0.807	12.6	*25*	NA	1	-4.03	4.83	4.10	4.26	*9*	0.16
1,2,4,5-Tetramethylbenzene	134.2	79.2	-0.795	3.48	*27*	5020	3.67	-4.02	4.82	4.08	4.10	*28*	0.02
Hexamethylbenzene	162.3	166.7	-0.774	0.235	*31*	4890	14.4	-4.68	5.43	4.61	4.61	*32*	0.00

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*23*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 4S. Predicted log K_{ow} values for anilines at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)	log $\overline{V}$ (L/mol)[a]	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Aniline	93.1	L[c]	-1.040	3.62E4	*34*	NA[d]	1	-0.410	1.45	1.13	1.09	*7*	-0.04
2-Toluidine	107.2	L	-0.968	1.63E4	*35*	NA	1	-0.817	1.78	1.42	1.42	*36*	0.00
3-Toluidine	107.2	L	-0.965	1.50E4	*35*	NA	1	-0.85	1.82	1.45	1.42	*37*	-0.03
N,N-Dimethylaniline	121.2	L	-0.895	1105	*35*	NA	1	-2.04	2.94	2.43	2.31	*18*	-0.12
2-Chloroaniline	127.6	L	-0.978	3765	*35*	NA	1	-1.53	2.51	2.06	1.90	*9*	-0.16
3-Chloroaniline	127.6	L	-0.979	5442	*35*	NA	1	-1.37	2.35	1.92	1.90	*9*	-0.02

[a] Molar volumes ($\overline{V}$) are obtained from liquid densities cited in Mackay et al. (*33*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 5S. Predicted log K_{ow} values for esters at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)	log $\overline{V}$ (L/mol)[a]	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Ethyl acetate	88.1	L[c]	-1.010	8.04E4	*34*	NA[d]	1	-0.040	1.05	0.78	0.73	*34*	-0.05
Propyl acetate	102.1	L	-0.939	2.04E4	*38*	NA	1	-0.699	1.64	1.29	1.24	*38*	-0.05
Butyl acetate	116.2	L	-0.881	6702	*38*	NA	1	-1.24	2.12	1.71	1.82	*38*	0.11
Ethyl acrylate	100.1	L	-0.965	1.5E4	*39*	NA	1	-0.824	1.79	1.43	1.33	*40*	-0.10
Methyl methacrylate	100.1	L	-0.974	1.6E4	*39*	NA	1	-0.796	1.77	1.41	1.38	*40*	-0.03
Methyl benzoate	136.1	L	-0.895	2100	*41*	NA	1	-1.81	2.71	2.23	2.14	*42*	-0.09
Ethyl benzoate	150.2	L	-0.845	720	*43*	NA	1	-2.32	3.16	2.63	2.64	*42*	0.01
Dimethyl phtahlate	194.2	L	-0.787	5000	*44*	NA	1	-1.59	2.38	1.92	1.86	*45*	-0.06
Diethyl phthalate	222.3	L	-0.704	1080	*46*	NA	1	-2.31	3.02	2.48	2.47	*47*	-0.01
Di-butyl phthalate	278.3	L	-0.575	13.0	*48*	NA	1	-4.33	4.91	4.14	4.08	*49*	-0.06
Di-octyl phthalate	390.6	L	-0.399	4.6E-4	*50*	NA	1	-8.93	9.33	8.02	8.10	*50*	0.08

[a] Molar volumes ($\overline{V}$) are obtained from liquid densities cited in Mackay et al. (*33*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC. [d] NA = not applicable for liquids.

Table 6S. Predicted log K_{ow} values for ethers at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Diethyl ether	74.1	L[c]	-0.984	6.03E4	*51*	NA	1	-0.090	1.07	0.80	0.83	*52*	0.03
Methyl-*t*-butyl ether	88.2	L	-0.925	5.16E4	*53*	NA	1	-0.23	1.16	0.86	0.94	*54*	0.08
Di-*n*-propyl ether	102.2	L	-0.861	2500	*53*	NA	1	-1.61	2.47	2.02	2.03	*34*	0.01
Di-*i*-propyl ether	102.2	L	-0.857	4900	*53*	NA	1	-1.32	2.18	1.76	1.52	*54*	-0.24
Tetrahydropyran	86.1	L	-1.008	8.57E4	*55*	NA	1	-2.0E-3	1.01	0.74	0.64	*54*	-0.10
Anisole	108.1	L	-0.964	2030	*55*	NA	1	-1.73	2.69	2.22	2.11	*18*	-0.11
Diphenyl ether	170.2	28	-0.800	18.0	*10*	4115	1.07	-3.95	4.75	4.02	4.08	*10*	0.06

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*1*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C.

Table 7S. Predicted log K_{ow} values for halogenated benzenes (HABZs) at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Fluorobenzene	96.1	L[c]	-1.027	1550	*25*	NA[d]	1	-1.79	2.82	2.34	2.27	*18*	-0.07
Chlorobenzene	112.6	L	-0.993	472	*56*	NA	1	-2.38	3.37	2.83	2.84	*18*	0.01
Bromobenzene	157.0	L	-0.979	410	*25*	NA	1	-2.58	3.56	2.99	2.99	*18*	0.00
Iodobenzene	204.0	L	-0.951	229	*57*	NA	1	-2.95	3.90	3.29	3.28	*38*	-0.01
1,2-Dichlorobenzene	147.0	L	-0.949	154	*35*	NA	1	-2.98	3.93	3.31	3.38	*26*	0.07
1,3-Dichlorobenzene	147.0	L	-0.943	124.5	*58*	NA	1	-3.07	4.01	3.39	3.44	*10*	0.05
1,4-Dichlorobenzene	147.0	53	-0.928	73	*35*	4350	1.88	-3.03	3.96	3.34	3.37	*26*	0.03
1,2,3-Trichlorobenzene	181.5	53	-0.903	16.3	*21*	4150	1.83	-3.79	4.69	3.98	4.04	*58*	0.06
1,2,4-Trichlorobenzene	181.5	L	-0.904	34.6	*21*	NA	1	-3.72	4.62	3.92	4.02	*35*	0.10
1,2,3,4-Tetrachlorobenzene	215.9	48	-0.848	3.42	*59*	4060	1.63	-4.59	5.43	4.63	4.60	*21*	-0.03
1,2,3,5-Tetrachlorobenzene	215.9	54.5	-0.848	3.23	*21*	4540	2.00	-4.53	5.37	4.58	4.59	*21*	0.01
1,2,4,5-Tetrachlorobenzene	215.9	140	-0.848	0.29	*59*	5760	15.0	-4.70	5.54	4.73	4.70	*21*	-0.03
Pentachlorobenzene	250.3	86	-0.781	0.385	*21*	4920	4.10	-5.20	5.98	5.11	5.03	*58*	-0.08
Hexachlorobenzene	284.8	228	-0.741	0.0050	*60*	6870	110	-5.71	6.46	5.52	5.50	*35*	-0.02

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*23*). Densities for tetrachlorobenzenes, pentachlorobenzene, and hexachlorobenzene are those of the liquids at their melting points (Chiou, *21*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 8S. Predicted log K_{ow} values for polycyclic aromatic hydrocarbons (PAHs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Indane	118.2	L[c]	-0.912	109	*62*	NA[d]	1	-3.04	3.95	3.33	3.33	*9*	0.00
Naphthalene	128.2	80	-0.903	31.7	*62*	4540	3.30	-3.09	3.99	3.36	3.36	*63*	0.00
1-Methylnaphthalene	142.2	L	-0.857	28.5	*62*	NA	1	-3.70	4.55	3.86	3.87	*9*	0.01
2-Methylnaphthalene	142.2	34	-0.860	25.4	*62*	2890	1.15	-3.69	4.55	3.85	3.86	*9*	0.01
1,3-Dimethylnaphthalene	156.2	L	-0.812	8.00	*62*	NA	1	-4.29	5.10	4.34	4.42	*9*	0.08
1,4-Dimethylnaphthalene	156.2	L	-0.813	11.4	*62*	NA	1	-4.14	4.95	4.20	4.37	*9*	0.17
1,5-Dimethylnaphthalene	156.2	82	-0.813	2.74	*64*	4790	3.67	-4.19	5.00	4.25	4.38	*9*	0.13
2,6-Dimethylnaphthalene	156.2	110	-0.818	0.997	*65*	5800	8.79	-4.25	5.07	4.31	4.31	*9*	0.00
1-Ethylnaphthalene	156.2	L	-0.810	10.0	*66*	NA	1	-4.19	5.00	4.25	4.39	*67*	0.14
2-Ethylnaphthalene	156.2	L	-0.803	7.97	*64*	NA	1	-4.29	5.10	4.33	4.38	*68*	0.05
1,4,5-Trimethylnaphthalene	170.2	L	-0.760	2.1	*62*	NA	1	-4.91	5.67	4.83	4.87	*69*	0.04
4-Methylbiphenyl	168.2	50	-0.817	4.05	*70*	4360	1.77	-4.37	5.19	4.41	4.63	*71*	0.22
4,4'-Dimethylbiphenyl	182.3	125	-0.656	0.175	*70*	5370	9.77	-5.03	5.68	4.83	5.09	*71*	0.26
Diphenylmethane	188.2	L	-0.728	14.1	*25*	NA	1	-4.13	4.85	4.11	4.14	*9*	0.03
Acenaphthene	154.2	96.2	-0.830	3.93	*62*	4950	5.01	-3.89	4.72	4.00	3.92	*72*	-0.08
Fluorene	166.2	116	-0.814	1.90	*73*	4670	6.33	-4.14	4.95	4.21	4.18	*69*	-0.03
Phenanthrene	178.2	101	-0.773	1.29	*74*	4450	4.60	-4.48	5.25	4.46	4.46	*9*	0.00

Anthracene	178.2	216	-0.800	0.0446	*75*	6900	94.7	-4.63	5.43	4.62	4.54	*63*	-0.08
9-Methylanthracene	192.3	81.5	-0.743	0.261	*62*	4790	3.63	-5.31	6.05	5.17	5.07	*63*	-0.10
Pyrene	202.3	156	-0.753	0.135	*62*	5620	18.1	-4.92	5.67	4.83	4.88	*9*	0.05
Fluoranthene	202.3	111	-0.746	0.260	*62*	4530	5.55	-5.15	5.89	5.03	5.16	*76*	0.13
Benz(a)anthracene	228.3	159	-0.694	0.014	*62*	5830	21.2	-5.89	6.58	5.63	5.61	*77*	-0.02
Benzo(a)pyrene	252.3	176.5	-0.651	1.21E-3	*78*	6070	31.6	-6.82	7.47	6.41	6.34	*79*	-0.07

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*61*). For solid compounds with m.p. > 100 °C, the supercooled liquid density is assumed to be 0.90 times the solid density. The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 9S. Predicted log K_{ow} values for polychlorinated biphenyls (PCBs) at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Biphenyl	154.2	71	-0.749	6.71	*58*	4180	2.57	-3.95	4.70	3.97	4.04	*10*	0.07
2-PCB	188.7	34	-0.717	4.13	*60*	3660	1.20	-4.58	5.30	4.50	4.51	*80*	0.01
3-PCB	188.7	L[c]	-0.717	3.63	*81*	NA[d]	1	-4.72	5.43	4.62	4.58	*82*	-0.04
4-PCB	188.7	78	-0.717	1.21	*83*	4740	3.35	-4.67	5.39	4.58	4.61	*84*	0.03
2,2'-PCB	223.1	61	-0.674	0.79	*60*	4510	2.27	-5.09	5.77	4.91	4.90	*82*	-0.01
2,4'-PCB	223.1	46	-0.674	0.637	*78*	4310	1.61	-5.34	6.01	5.13	5.10	*80*	-0.03
2,5-PCB	223.1	L	-0.674	1.12	*83*	NA	1	-5.30	5.98	5.09	5.16	*58*	0.07
2,6-PCB	223.1	36	-0.674	1.39	*58*	3010	1.20	-5.13	5.80	4.94	4.93	*58*	-0.01
3,3'-PCB	223.1	29	-0.674	0.354	*83*	4080	1.10	-5.76	6.43	5.50	5.30	*84*	-0.20
4,4'-PCB	223.1	149	-0.674	0.0363	*83*	5700	16.9	-5.56	6.24	5.32	5.33	*82*	0.01
2,2',5-PCB	257.5	44	-0.649	0.248	*78*	4280	1.54	-5.83	6.48	5.53	5.60	*82*	0.07
2,4,4'-PCB	257.5	58	-0.649	0.116	*21*	4470	2.12	-6.02	6.67	5.70	5.62	*21*	-0.08
2,4,5-PCB	257.5	79	-0.649	0.092	*60*	5450	4.10	-5.83	6.48	5.54	5.51	*58*	-0.03
2,4,6-PCB	257.5	63	-0.649	0.226	*58*	3940	2.12	-5.73	6.38	5.45	5.47	*58*	0.02
2,2',3,3'-PCB	292.0	121	-0.615	0.0156	*82*	5320	8.92	-6.32	6.94	5.94	5.80	*21*	-0.14
2,3,4,5-PCB	292.0	92	-0.615	0.0209	*78*	6020	6.46	-6.33	6.95	5.95	5.72	*58*	-0.23
2,2',5,5'-PCB	292.0	87	-0.615	0.046	*85*	4860	4.11	-6.19	6.80	5.82	5.81	*21*	-0.01

2,2',4,5,5'-PCB	326.4	77	-0.593	0.0103	*78*	4490	3.09	-7.01	7.61	6.52	6.50	*82*	-0.02
2,3,4,5,6-PCB	326.4	124	-0.593	5.48E-3	*58*	5210	8.97	-6.82	7.42	6.36	6.30	*58*	-0.06
2,2',3,3',4,4'-PCB	360.9	150	-0.526	2.85E-4	*58*	6980	32.6	-7.59	8.12	6.97	6.98	*58*	0.01
2,2',3,3',6,6'-PCB	360.9	114	-0.526	4.51E-3	*86*	5070	7.16	-7.05	7.57	6.49	6.63	*58*	0.14
2,2',4,4',5,5'-PCB	360.9	104	-0.526	1.2E-3	*60*	5090	6.05	-7.70	8.22	7.06	6.90	*82*	-0.16
2,2',4,4',6,6'-PCB	360.9	114	-0.526	4.1E-4	*58*	4180	5.07	-8.24	8.77	7.54	7.55	*58*	0.01
2,2',3,3',4,4',6-PCB	395.3	122	-0.494	2.17E-3	*58*	4860	7.50	-7.39	7.88	6.75	6.66	*58*	-0.09
2,2',3,3',5,5',6,6'-PCB	429.8	162	-0.499	3.93E-4	*58*	5450	18.1	-7.78	8.28	7.11	7.11	*58*	0.00
2,2',3,3',4,5,5',6,6'-PCB	464.2	182	-0.467	1.8E-5	*58*	5410	23.4	-9.04	9.51	8.19	8.16	*58*	-0.03

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*23*). For solid compounds with m.p. > 100 ºC, the supercooled liquid density is assumed to be 0.90 times the solid density. The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC.. [d] NA = not applicable for liquids.

Table 10S. Predicted log K_{ow} values for dibenzodioxins-dibenzofurans (DDXDFs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Dibenzofuran	168.2	99	-0.812	4.22	*70*	4680	3.87	-4.01	4.83	4.09	4.17	*10*	0.08
2,8-Dichlorodibenzofuran	237.1	185	-0.739	0.0145	*70*	6020	34.9	-5.67	6.41	5.48	5.44	*71*	-0.04
1,2,4-Trichlorodibenzo-*p*-dioxin	287.5	129	-0.687	8.41E-3	*87*	8070	34.0	-6.00	6.69	5.73	5.57	*87*	-0.16
1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	322.0	189	-0.668	6.3E-4	*87*	7510	90.1	-6.75	7.42	6.37	6.20	*71*	-0.17
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin	322.0	306	-0.668	1.93E-5	*88*	9550	251	-6.82	7.49	6.43	6.64	*89*	0.21

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*61*). [b] $S_w = F_{sl} S_w^*$.

Table 11S. Predicted log K_{ow} values for heterocyclic compounds at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Indole	117.2	53	-0.958	3558	*27*	4400	1.89	-1.24	2.20	1.79	1.92	*7*	0.13
Quinoline	129.2	L[c]	-0.927	5426	*90*	NA[d]	1	-1.38	2.30	1.88	2.03	*91*	0.15
Carbazole	167.2	248	-0.830	1.03	*92*	7030	161	-3.00	3.83	3.21	3.29	*93*	0.08
Thiophene	84.1	L	-1.100	3015	*27*	NA	1	-1.45	2.55	2.11	1.82	*91*	-0.29
Benzo(b)thiophene	134.2	32	-0.933	130	*92*	4120	1.17	-2.94	3.88	3.26	3.26	*94*	0.00
Dibenzothiophene	184.3	100	-0.795	1.11	*92*	5170	6.94	-4.38	5.17	4.40	4.38	*95*	-0.02

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*33*). The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids.

Table 12S. Predicted log K_{ow} values for organochlorine pesticides (OGCLs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Lindane	290.9	113	-0.762	7.87	*97*	5640	8.77	-3.62	4.39	3.70	3.72	*98*	0.02
α-HCH	290.9	158	-0.762	1.21	*98*	7400	47.3	-3.71	4.47	3.77	3.81	*98*	0.04
Dieldrin	380.9	176	-0.616	0.468	*99*	4800	15.3	-4.73	5.35	4.53	4.55	*100*	0.02
Chlordane	409.8	107	-0.543	0.032	*101*	6700	12.0	-6.03	6.57	5.60	5.54	*102*	-0.06
Heptachlor	373.3	96	-0.645	0.056	*103*	5490	5.95	-6.05	6.69	5.72	5.73	*104*	0.01
p,p'-DDT	354.5	109	-0.603	0.0055	*60*	6300	10.4	-6.79	7.40	6.34	6.36	*35*	0.02
p,p'-DDE	319.0	88.5	-0.627	0.040	*105*	5800	5.59	-6.15	6.78	5.80	5.77	*106*	-0.03

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*96*). For solid compounds with m.p. > 100 ºC, the supercooled liquid density is assumed to be 0.90 times the solid density. [b] $S_w = F_{sl} S_w^*$.

Table 13S. Predicted log K_{ow} values for organophosphate pesticides (OGPPs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Trichlorfon	257.4	84	-0.827	1.2E5	*107*	4820	3.84	0.25	0.57	0.34	0.43	*108*	0.09
Dimethoate	229.3	52	-0.743	3.9E4	*109*	4400	1.89	-0.49	1.24	0.91	0.79	*37*	-0.12
Chlorfenvinphos	359.6	L[c]	-0.578	145	*109*	NA[d]	1	-3.39	3.97	3.31	3.23	*110*	-0.08
Phorate	260.4	L	-0.647	22	*111*	NA	1	-4.07	4.72	3.98	3.92	*107*	-0.06
Methyl parathion	263.5	36	-0.712	60	*112*	4170	1.29	-3.53	4.25	3.57	3.32	*9*	-0.25
Parathion	291.3	L	-0.638	24	*113*	NA	1	-4.08	4.72	3.98	3.81	*105*	-0.17
Diazinon	304.4	L	-0.562	40	*114*	NA	1	-3.88	4.44	3.73	3.81	*108*	0.08
Disulfon	274.4	L	-0.619	25	*109*	NA	1	-4.04	4.66	3.92	4.02	*108*	0.10
Turbufos	288.4	L	-0.583	5.07	*115*	NA	1	-4.75	5.34	4.51	4.48	*108*	-0.03
Fonofos	246.3	L	-0.673	15.7	*108*	NA	1	-4.20	4.87	4.11	3.89	*108*	-0.22
Ethion	384.5	L	-0.501	1.1	*108*	NA	1	-5.54	6.04	5.13	5.07	*108*	-0.06
Ronnel	321.6	41	-0.663	1.08	*105*	4240	1.44	-5.32	5.98	5.09	4.88	*105*	-0.21
Chlorpyrifos	350.6	43	-0.601	0.40	*105*	6200	1.82	-5.68	6.29	5.36	5.27	*76*	-0.09
Leptophos	412.1	72	-0.570	0.021	*108*	4660	2.92	-6.83	7.40	6.34	6.31	*105*	-0.03

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*96*). The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC. [d] NA = not applicable for liquids.

Table 14S. Predicted log K_{ow} values for carbamate pesticides at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Oxamyl	219.3	102	-0.646	2.83E5	*37*	5060	5.78	0.87	-0.23	-0.39	-0.43	*116*	-0.04
Methomyl	162.2	79	-0.902	5.8E4	*117*	4750	3.42	0.088	0.81	0.56	0.60	*47*	0.04
Propoxur	209.2	91.5	-0.725	1860	*108*	4920	4.55	-1.39	2.12	1.69	1.55	*108*	-0.14
Aldicarb	190.2	100	-0.798	6016	*37*	6200	8.21	-0.59	1.38	1.05	1.13	*108*	0.08
Aminocarb	208.3	94	-0.703	1360	*118*	4950	4.82	-1.50	2.20	1.76	1.73	*108*	-0.03
Carbaryl	201.2	142	-0.742	104	*108*	5800	15.8	-2.09	2.83	2.32	2.31	*108*	-0.01
Methiocarb	225.3	119	-0.693	30	*117*	5290	8.52	-2.95	3.64	3.03	2.92	*37*	-0.11
Carbofuran	221.3	152	-0.680	480	*119*	5740	18.1	-1.41	2.09	1.66	1.63	*120*	-0.03
Chlorpropham	213.7	41.4	-0.742	102.3	*121*	4900	1.54	-3.13	3.87	3.24	3.06	*122*	-0.18
Fenoxycarb	301.3	54	-0.611	5.7	*107*	4410	1.94	-4.44	5.05	4.26	4.30	*107*	0.04

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*96*). For solid compounds with m.p. > 100 ºC. the supercooled liquid density is assumed to be 0.90 times the solid density. The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$.

Table 15S. Predicted log K_{ow} values for amide-urea-triazine pesticides (AUTZs) at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Alachlor	269.8	41	-0.623	240	*123*	4240	1.44	-2.89	3.52	2.91	2.92	*30*	0.01
Metolachlor	283.8	L[c]	-0.596	488	*124*	NA[d]	1	-2.76	3.36	2.77	2.90	*124*	0.13
Propanil	218.1	93	-0.758	130	*125*	4800	4.51	-2.57	3.33	2.76	2.80	*37*	0.04
Fenuron	164.2	133	-0.838	3700	*126*	5800	13.5	-0.52	1.35	1.03	0.96	*37*	-0.07
Chlorotoluron	212.7	148	-0.773	80.6	*127*	5680	16.5	-2.20	2.98	2.45	2.41	*37*	-0.04
Linuron	249.1	95	-0.701	75	*128*	6850	9.03	-2.57	3.27	2.70	2.76	*37*	0.06
Monolinuron	214.6	81.5	-0.748	580	*129*	4790	3.63	-2.01	2.76	2.26	2.30	*37*	0.04
Neburon	275.2	103	-0.657	4.8	*130*	5080	5.92	-3.99	4.64	3.91	4.10	*131*	0.19
Diuron	233.1	159	-0.729	37.3	*132*	5830	21.2	-2.47	3.20	2.64	2.68	*37*	0.04
Ametryn	227.4	86	-0.719	195	*133*	4820	3.84	-2.48	3.20	2.65	2.61	*131*	-0.04
Atrazine	215.7	175	-0.741	30	*126*	6050	30.5	-2.37	3.11	2.57	2.64	*134*	0.07
Cyanzine	240.7	167	-0.698	171	*129*	5940	25.4	-1.74	2.44	1.97	2.04	*131*	0.07
Simazine	201.7	227	-0.764	15.1	*135*	6750	100	-2.13	2.89	2.38	2.27	*136*	-0.11
Prometon	225.3	92	-0.684	750	*129*	4930	4.61	-1.81	2.50	2.02	1.94	*136*	-0.08

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*96*). For solid compounds with m.p. > 100 ºC, the supercooled liquid density is assumed to be 0.90 times the solid density. The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC. [d] NA = not applicable for liquids.

Table 16S. Predicted log K_{ow} values for phenols at 25 °C from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (°C)[a]	log $\overline{V}$ (L/mol)	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)[a]	F_{sl}	log S_w (mol/L)[b]	log K^o_{sw}	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
Phenol	94.1	41	-1.051	7.65E4	*38*	2750	1.27	0.0129	1.04	0.78	1.45	*38*	0.67
o-Cresol	108.1	L[c]	-1.021	2.68E4	*137*	NA[d]	1	- 0.61	1.63	1.29	1.96	*38*	0.67
m-Cresol	108.1	L	-0.982	1.96E4	*137*	NA	1	- 0.74	1.72	1.37	1.96	*38*	0.59
2,4-Dimethylphenol	122.2	L	-0.928	8200	*137*	NA	1	-1.17	2.10	1.70	2.34	*38*	0.64
2,6-Dimethylphenol	122.2	49	-0.967	6150	*137*	4350	1.73	-1.06	2.03	1.64	2.31	*38*	0.67
2-Ethylphenol	122.2	L	-0.929	1.40E4	*137*	NA	1	-0.94	1.87	1.50	2.47	*9*	0.97
2,4,6-Trimethylphenol	136.2	72	-0.907	1007	*138*	4660	2.92	-1.67	2.57	2.11	2.73	*38*	0.62
2-Chlorophenol	128.6	L	-0.990	1.15E4	*10*	NA	1	-1.05	2.04	1.65	2.15	*18*	0.50
2,4-Dichlorophenol	163.0	45	-0.929	4500	*139*	4290	1.58	-1.36	2.29	1.86	3.08	*9*	1.22
2,4,5-Trichlorophenol	197.5	65	-0.881	649	*140*	4560	2.49	-2.09	2.97	2.46	3.72	*9*	1.26
2,3,4,6-Tetrachlorophenol	231.9	70	-0.839	183	*138*	4630	2.79	-2.66	3.50	2.92	4.24	*141*	1.32
Pentachlorophenol	266.3	190	-0.825	8	*142*	6250	43.0	-2.89	3.71	3.11	4.84	*143*	1.73
2-Naphthol	144.2	122	-0.902	754	*144*	4490	6.44	-1.47	2.37	1.94	2.84	*145*	0.90
4-Octylphenol	206.3	42	-0.685	12.6	*146*	4250	1.47	-4.05	4.73	3.99	4.12	*147*	0.13
Nonylphenol-4EOs[e]	396.2	L	-0.411	7.65	*146*	NA	1	-4.71	5.12	4.31	4.24	*148*	-0.07

[a] Melting points (m.p.), molar heats of fusion ($\Delta\overline{H}_f$), and densities (for calculation of $\overline{V}$) are from those cited in Mackay et al. (*33*). For solid compounds with m.p. > 100 °C, the supercooled liquid density is assumed to be 0.90 times the solid density. The underlined $\Delta\overline{H}_f$ values are estimated with $\Delta\overline{H}_f = 13.5\ T_m$. [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 °C. [d] NA = not applicable for liquids. [e] 4EOs = four ethylene-oxide units

Table 17S. Predicted log K_{ow} values for alcohols at 25 ºC from respective S_w and $\overline{V}$ data

Compound	M (g/mol)	m.p. (ºC)	log $\overline{V}$ (L/mol)[a]	S_w^* (mg/L)	Ref	$\Delta\overline{H}_f$ (cal/mol)	F_{sl}	log S_w (mol/L)[b]	log K_{sw}^o	Pred. log K_{ow}	Expt. log K_{ow}	Ref	Δ log K_{ow}
1-Butanol	74.1	L[c]	-1.039	7.32E4	*149*	NA[d]	1	-0.0053	1.04	0.78	0.89	*9*	0.11
1-Pentanol	88.2	L	-0.965	2.21E4	*149*	NA	1	-0.60	1.57	1.23	1.53	*38*	0.30
1-Hexanol	102.2	L	-0.903	5838	*150*	NA	1	-1.24	2.15	1.73	2.03	*9*	0.30
1-Heptanol	116.2	L	-0.849	1676	*150*	NA	1	-1.84	2.69	2.21	2.57	*38*	0.36
1-Octanol	130.2	L	-0.801	495	*151*	NA	1	-2.42	3.22	2.67	3.15	*52*	0.48
Benzyl alcohol	108.2	L	-0.983	3.8E4	*152*	NA	1	-0.45	1.44	1.12	1.10	*18*	-0.02

[a] Molar volumes ($\overline{V}$) are obtained from liquid densities cited in Mackay et al. (*33*). [b] $S_w = F_{sl} S_w^*$. [c] Liquids at 25 ºC. [d] NA = not applicable for liquids.

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