Supporting Information for:

Predicting Air-Water Adsorption Coefficients Using Universal Solvation and Surface Area Models

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TABLE S1. Experimental and Calculated $\Delta G^{\circ}_{org/a}$ Values for the SM5.0R Phosphorus Data Set.

		$\Delta G^{\circ}_{org/a}$ (kcal/mole)	
Solute	Solvent[a]	SM5.0R[b]	Expt.
trimethylphosphate	1	-5.01	-8.02
	2	-5.74	-7.24
	3	-5.58	-9.74
	4	-4.41	-5.67
	5	-4.92	-8.55
	6	-4.43	-5.59
	7	-4.44	-5.82
	8	-4.67	-7.81
triethylphosphate	1	-7.70	-8.58
	2	-8.72	-7.51
	3	-8.39	-10.90
	4	-6.83	-7.60
	5	-7.49	-9.59
	6	-6.84	-6.67
	7	-6.85	-6.78
	8	-6.94	-8.88
tripropylphosphate	1	-9.81	-9.34
	2	-11.14	-8.60

	3	-10.66	-11.11
	4	-8.71	-7.71
	6	-8.72	-7.50
	7	-8.74	-7.24
	8	-8.67	-8.65
dimethyl methylphosphonate	9	-2.85	-5.43
2,2-dichloroethenyl dimethyl phosphate	1	-6.19	-9.09
	8	-14.76	-8.59
methyl 3-methyl-4-thiomethoxyphenyl thiophosphate	8	-16.36	-12.55
diethyl 2,4-dichlorophenyl thiophosphate	8	-9.45	-10.87
dimethyl 4-nitrophenyl thiophosphate	1	-12.22	-9.21
	3	-13.47	-9.51
	8	-12.29	-11.70
O-ethyl O'-4-bromo-2-chlorophenyl S-propyl phosphorothioate	8	-13.73	-10.49
dimethyl 2,4,5-trichlorophenyl thiophosphate	8	-9.78	-11.69
dimethyl 4-bromo-2,5-dichlorophenyl thiophosphate	8	-10.96	-12.30
diethyl 4-nitrophenyl thiophosphonate	1	-13.95	-8.58
	8	-13.77	-11.31
ethyl 4-cyanophenyl phenylthiophosphonate	8	-15.26	-11.06

[a](1) benzene (2) tetrachlormethane (3) trichloromethane (4) cyclohexane (5) dichloroethane (6) *n*-heptane (7) *n*-hexane (8) 1-octanol (9) *n*-hexadecane. [b]Calculated with optimized surface tension coefficient for phosphorus.

TABLE S2. Experimental Data Used to Parameterize Equation 2.

Solute	$\Delta H_{i/a}$ (kcal/mole)[a]	ln $K_{i/a}$ (288 K)[b]
Z-2-octene	-8.6	-13.25
E-2-octene	-8.6	-13.25
benzene	-7.5	-14.16
toluene	-8.9	-13.16
ethylbenzene	-9.9	-12.31
di-*n*-propyl ether	-12.8	-10.36
ethyl formate	-6.9	-13.97
fluorobenzene	-7.8	-13.96
chlorobenzene	-8.4	-13.13
1,2-dichloroethane	-7.8	-13.58
dichloromethane	-5.6	-14.98
trichloromethane	-6.4	-14.41
tetrachloromethane	-5.6	-15.17

[a]Experimental values, taken from ref. 24. [b]Taken from i/a data set; adjusted to 288 K using experimental $\Delta H_{i/a}$ values given in this table.

TABLE S3. Calculated and Experimental $K_{a/w}$ Values for the Solutes in the EC test set.

		SM5.42R			SM5.43R	
Solute	SM5.0R	AM1	HF/MIDI![a]	HF/6-31G(d)	*m*PW1PW91/6-31G(d)	Expt.
EPTC	-4.03	-3.31	-2.15	-2.24	-0.92	-2.51
alachlor	-5.92	-3.79	-3.66	-3.56	-2.42	-5.94
atrazine	-8.07	-6.39	-7.64	-7.40	-7.80	-6.78
benfluralin	-4.26	-0.05	-1.34	-0.85	0.73	-0.92 / -3.11
cyanazine	-10.90	-6.41	-9.15	-8.94	-7.69	-9.95
desmetryn	-9.81	-8.07	-8.56	-8.34	-9.06	-7.57
diazinon	-13.42	-4.46	-4.48	-5.06	-3.24	-4.74
ethoprop	-9.35	3.34	0.51[b]	-0.55	-3.19[c]	-5.18
metamitron	-12.01	-8.77	-9.96	-10.19	-7.54	-10.27
metolachlor	-5.27	-3.39	-3.78	-3.45	-2.62	-6.33
pendimethalin	-6.08	-3.06	-3.63	-3.42	-2.07	-3.28
prometryn	-9.32	-6.91	-7.44	-7.11	-7.23	-6.43
propachlor	-5.17	-5.48	-4.95	-5.27	-4.18	-5.31
simazine	-8.52	-7.04	-8.32	-8.15	-8.82	-6.94
terbutryn	-8.87	-6.82	-7.15	-6.89	-7.24	-5.66
trifluralin	-4.89	-0.32	-1.79	-1.09	0.84	-2.52
1,2,4-trichlorobenzene	-0.72	-0.95	-1.30	-0.97	-0.89	-0.95
1,2,3,5-tetrachlorobenzene	-0.76	-0.53	-1.09	-0.67	-0.60	-1.34
PCB, 2,4,5-	-1.68	-1.23	-2.04	-1.53	-1.32	-2.05
PCB, 2,2',3,4,5'-	-1.75	-1.23	-2.38	-1.64	-1.39	-2.06
PCDD, 2,3,7,8-	-6.39	-3.09	-3.92	-3.11	-2.51	-2.8
PCDD, 1,2,3,4,7-	-5.91	-2.76	-3.51	-2.66	-1.96	-3.58
phenanthrene	-2.37	-3.55	-3.04	-2.86	-2.70	-2.83
benzo(a)pyrene	-3.89	-5.81	-4.78	-4.40	-4.08	-4.73
MUEL[d]	1.88	1.32	0.95	0.91	1.51	

[a]This is the model that was used to calculate the $K_{a/w}$ and $K_{h/a}$ values given in Table 7. [b]This value was not given in Table 7, nor was it used in the STSA model. [c]This value is given in Table 7, and was used in the STSA model. [d]Mean unsigned error in the logarithm of $K_{a/w}$ over 23 solutes (benfluralin excluded).

END OF SUPPORTING INFORMATION