Supplementary Material (ESI) for Journal of Environmental Monitoring

Solvation parameters for mercury and mercury(II) compounds: calculation of properties of environmental interest

Michael H. Abraham, Javier Gil-Lostes, William E. Acree, Jr., J. Enrique Cometto-Muñiz, and William S. Cain.

Supplementary Material

Tables S1 to S5

Table S1 Coefficients in equations for water to solvent and gas to solvent partitions, at 298K [a]

Process	SP	*c*	*e*	*s*	*a*	*b*	*l*	*v*
Water to :								
Octanol	log Ps	0.088	0.562	-1.054	0.034	-3.460	0	3.814
Isobutanol	log Ps	0.249	0.480	-0.639	-0.050	-2.284	0	2.758
Pentanol	log Ps	0.175	0.575	-0.787	0.020	-2.837	0	3.249
Hexanol	log Ps	0.143	0.718	-0.980	0.145	-3.214	0	3.403
Decanol	log Ps	0.008	0.485	-0.974	0.015	-3.798	0	3.945
Dichloromethane	log Ps	0.314	0.001	0.022	-3.238	-4.137	0	4.259
Trichloromethane	log Ps	0.327	0.157	-0.391	-3.191	-3.437	0	4.191
Tetrachloromethane	log Ps	0.260	0.573	-1.254	-3.558	-4.588	0	4.589
1,2-Dichloroethane	log Ps	0.227	0.278	-0.167	-2.816	-4.324	0	4.205
Pentane	log Ps	0.369	0.386	-1.568	-3.535	-5.215	0	4.514
Hexane	log Ps	0.361	0.579	-1.723	-3.599	-4.764	0	4.344
Heptane	log Ps	0.325	0.670	-2.061	-3.317	-4.733	0	4.543
Octane	log Ps	0.223	0.642	-1.647	-3.480	-5.067	0	4.526
Nonane	log Ps	0.240	0.619	-1.713	-3.532	-4.921	0	4.482
Decane	log Ps	0.160	0.585	-1.734	-3.435	-5.078	0	4.582
Hexadecane	log Ps	0.087	0.667	-1.617	-3.587	-4.869	0	4.433
Cyclohexane	log Ps	0.159	0.784	-1.678	-3.740	-4.929	0	4.577
Methylcyclohexane	log Ps	0.246	0.782	-1.982	-3.517	-4.293	0	4.528
Isooctane	log Ps	0.288	0.382	-1.668	-3.639	-5.000	0	4.561

Benzene	log Ps	0.142	0.464	-0.588	-3.099	-4.625	0	4.491
Toluene	log Ps	0.143	0.527	-0.720	-3.010	-4.824	0	4.545
Chlorobenzene	log Ps	0.040	0.246	-0.462	-3.038	-4.769	0	4.640
Bromobenzene	log Ps	-0.130	0.394	-0.280	-3.331	-4.640	0	4.583
Iodobenzene	log Ps	-0.181	0.410	-0.334	-3.300	-4.595	0	4.549
Nitrobenzene	log Ps	-0.181	0.576	0.003	-2.356	-4.420	0	4.263
Diethyl ether	log Ps	0.248	0.561	-1.016	-0.226	-4.553	0	4.075
Diisopropylether	log Ps	0.197	0.695	-1.220	-0.238	-4.921	0	4.388
Dibutylether	log Ps	0.252	0.677	-1.506	-0.807	-5.249	0	4.815
Ethyl acetate	log Ps	0.253	1.157	-1.397	-0.054	-3.755	0	3.726
Butyl acetate	log Ps	-0.468	0.712	-0.397	0.010	-3.743	0	3.865
Olive oil	log Ps	-0.011	0.577	-0.800	-1.470	-4.921	0	4.173
Tributylphosphate	log Ps	0.015	0.804	-0.862	1.389	-4.647	0	4.129
Carbon disulfide	log Ps	0.047	0.686	-0.943	-3.603	-5.818	0	4.921
Methanol/Dry	log Ps	0.329	0.299	-0.671	0.080	-3.389	0	3.512
Ethanol/Dry	log Ps	0.208	0.409	-0.959	0.186	-3.645	0	3.928
Propanol/Dry	log Ps	0.148	0.436	-1.098	0.389	-3.893	0	4.036
Butanol/Dry	log Ps	0.152	0.438	-1.177	0.096	-3.919	0	4.122
Pentanol/Dry	log Ps	0.080	0.521	-1.294	0.208	-3.908	0	4.208
Hexanol/Dry	log Ps	0.044	0.470	-1.153	0.083	-4.057	0	4.249
Heptanol/Dry	log Ps	-0.026	0.491	-1.258	0.035	-4.155	0	4.415
Octanol/Dry	log Ps	-0.034	0.490	-1.048	-0.028	-4.229	0	4.219
Decanol/Dry	log Ps	-0.062	0.754	-1.461	0.063	-4.053	0	4.293
Isopropanol/Dry	log Ps	0.063	0.320	-1.024	0.445	-3.824	0	4.067
Trifluoroethanol/Dry	log Ps	0.368	-0.505	-0.677	-1.756	-0.325	0	3.123
Ethyl acetate/Dry	log Ps	0.358	0.362	-0.449	-0.668	-5.016	0	4.155
Propanone/Dry	log Ps	0.335	0.349	-0.231	-0.411	-4.793	0	3.963
Butanone/Dry	log Ps	0.354	0.003	-0.164	-0.979	-4.706	0	4.160
Dimethylformamide/Dry	log Ps	0.105	0.317	0.462	1.154	-4.843	0	3.757
Acetonitrile/Dry	log Ps	0.413	0.077	0.326	-1.566	-4.391	0	3.364
Nitromethane/Dry	log Ps	0.023	-0.091	0.793	-1.463	-4.364	0	3.460
DMSO/ Dry	log Ps	-0.231	0.520	0.757	1.799	-4.652	0	3.428
Dibutyl ether/Dry	log Ps	0.203	0.369	-0.954	-1.488	-5.426	0	4.508
Gas to water	logKw	-0.994	0.577	2.549	3.813	4.841	0	-0.869
Gas to:								
Octanol	log Ks	-0.198	0.002	0.709	3.519	1.429	0.858	0
Dichloromethane	log Ks	0.121	-0.450	1.677	0.404	0.786	0.940	0
Trichloromethane	log Ks	0.116	-0.467	1.203	0.138	1.432	0.994	0
Tetrachloromethane	log Ks	0.282	-0.303	0.460	0.000	0.000	1.047	0

1,2-Dichloroethane	log Ks	0.011	-0.150	1.436	0.649	0.736	0.936	0
Pentane	log Ks	0.335	-0.276	0.000	0.000	0.000	0.968	0
Hexane	log Ks	0.292	-0.169	0.000	0.000	0.000	0.979	0
Heptane	log Ks	0.275	-0.162	0.000	0.000	0.000	0.983	0
Octane	log Ks	0.215	-0.049	0.000	0.000	0.000	0.967	0
Nonane	log Ks	0.200	-0.145	0.000	0.000	0.000	0.980	0
Decane	log Ks	0.156	-0.143	0.000	0.000	0.000	0.989	0
Hexadecane	log Ks	0.000	0.000	0.000	0.000	0.000	1.000	0
Cyclohexane	log Ks	0.163	-0.110	0.000	0.000	0.000	1.013	0
Methylcyclohexane	log Ks	0.318	-0.215	0.000	0.000	0.000	1.012	0
Isooctane	log Ks	0.275	-0.244	0.000	0.000	0.000	0.972	0
Benzene	log Ks	0.107	-0.313	1.053	0.457	0.169	1.020	0
Toluene	log Ks	0.121	-0.222	0.938	0.467	0.099	1.012	0
Chlorobenzene	log Ks	0.053	-0.553	1.254	0.364	0.000	1.041	0
Nitrobenzene	log Ks	-0.273	0.039	1.803	1.231	0.000	0.929	0
Diethyl ether	log Ks	0.245	-0.360	1.079	3.316	0.000	0.889	0
Isopropyl ether	log Ks	0.114	-0.032	0.685	3.108	0.000	0.941	0
Dibutylether	log Ks	0.145	0.074	0.250	2.621	0.000	1.019	0
Olive oil	log Ks	-0.230	0.009	0.795	1.353	0.000	0.888	0
Carbon disulfide	log Ks	0.101	0.251	0.177	0.027	0.095	1.068	0
Methanol/ Dry	log Ks	-0.004	-0.215	1.173	3.701	1.432	0.769	0
Ethanol/ Dry	log Ks	0.012	-0.206	0.789	3.635	1.311	0.853	0
Propanol/ Dry	log Ks	-0.028	-0.185	0.648	4.022	1.043	0.869	0
Butanol/Dry	log Ks	-0.039	-0.276	0.539	3.781	0.995	0.934	0
Pentanol/ Dry	log Ks	-0.042	-0.277	0.526	3.779	0.983	0.932	0
Hexanol/ Dry	log Ks	-0.035	-0.298	0.626	3.726	0.729	0.936	0
Heptanol/Dry	log Ks	-0.062	-0.168	0.429	3.541	1.181	0.927	0
Octanol/ Dry	log Ks	-0.120	-0.203	0.560	3.576	0.702	0.939	0
Decanol/ Dry	log Ks	-0.136	-0.038	0.325	3.674	0.767	0.947	0
Isopropanol/ Dry	log Ks	-0.060	-0.335	0.702	4.017	1.040	0.893	0
Trifluoroethanol/ Dry	log Ks	-0.133	-0.611	1.457	1.899	4.461	0.633	0
Ethyl acetate/ Dry	log Ks	0.203	-0.335	1.251	2.949	0.000	0.917	0
Propanone/ Dry	log Ks	0.154	-0.277	1.522	3.258	0.078	0.863	0
Dimethylformamide/Dry	log Ks	-0.161	-0.189	2.327	4.756	0.000	0.808	0
Acetonitrile/ Dry	log Ks	-0.007	-0.595	2.461	2.085	0.418	0.738	0
Nitromethane/ Dry	log Ks	-0.340	-0.297	2.689	2.193	0.514	0.728	0
DMSO/ Dry	log Ks	-0.619	0.131	2.811	5.474	0.000	0.734	0
Dibutylether/Dry	log Ks	0.165	-0.421	0.760	2.102	-0.664	1.002	0
Gas to water	log Kw	-1.271	0.822	2.743	3.904	4.814	-0.213	0

[a] Solvents are wet (i.e. saturated with water) unless shown as ‘Dry’.

Table S2 Solubilities of mercury(II) chloride at 298K, and derived log Ps and log Ks values

Solvent	Log Ss [34]	Log Ss [35]	Log Ps	Log Ks
Water	-0.57 [2]			8.02
Hexane	-3.80		-3.23	4.79
Heptane	-3.92		-3.35	4.67
Decane	-4.05		-3.48	4.54
Dodecane	-3.95		-3.38	4.64
Cyclohexane	-3.72		-3.15	4.87
Benzene	-1.66	-1.80	-1.16	6.86
Toluene	-1.62		-1.05	6.97
Ether		-0.77	-0.20	(7.82)
Propanone		0.51	(1.08)	
Acetonitrile		0.26	0.83	8.85
Methanol		0.30	(0.87)	
DMSO		0.30	(0.87)	
Wet octanol			-0.22 [9]	7.80
Wet ether			-0.58 [9]	7.44
Wet pentanol			0.25 [36]	8.27
Wet benzene			-1.08 [36]	6.94
Wet toluene			-1.12 [36]	6.90

Table S3 Solubilities of mercury(II) bromide at 298K and derived log Ps and log Ks values.

Solvent	Log Ss [34]	Log Ss [35]	Log Ps	Log Ks
Water	-1.77 [2]			7.04
Hexane	-3.52		1.75	5.29
Heptane	-3.62		1.85	5.19
Decane	-3.68		1.91	5.13
Dodecane	-3.68		1.91	5.13
Cyclohexane	-3.35		1.58	5.46
Benzene	-1.68	-1.80	-0.09, 0.03	7.13
Toluene	-1.64		-0.13	7.17
Ether		-1.17	-0.60	7.64
Propanone		(-0.02)		
Acetonitrile		-0.59	1.18	8.22
Methanol		(0.18)		
DMSO		(0.51)		
Dioxane	(-1.05)			

Table S4 Solubilities of mercury(II) iodide at 298K and derived log Ps and log Ks values

Solvent	Log Ss [34]	Log Ss [35]	Log Ps	Log Ks
Water	-3.92 [2]			5.69
Hexane	-3.38		0.54	6.23
Heptane	-3.52		0.40	6.09
Decane	-3.62		0.30	5.99
Cyclohexane	-3.23		0.69	6.38
Benzene	-2.21	-2.12	1.71, 1.80	7.44
Toluene	-2.11		1.81	7.50
Ether		-2.08	1.84	7.53
Dioxane	(-0.98)			
Propanone		-1.51	2.41	8.10
Acetonitrile		-2.12	1.80	7.49
Methanol		(-1.17)		
DMSO		(0.63)		

Table S5 Predicted values of log Kw for organomercury(II) compounds from 273 to 373K

Species/ T:	298	273	293	303	323	343	353	363	373
MeHgCl	4.72	5.41	4.84	4.60	4.18	3.84	3.69	3.55	3.43
EtHgCl	4.58	5.32	4.71	4.45	4.01	3.66	3.51	3.37	3.26
PrHgCl	4.46	5.26	4.60	4.33	3.86	3.50	3.35	3.22	3.10
BuHgCl	4.34	5.21	4.49	4.20	3.71	3.33	3.18	3.05	2.94
PeHgCl	4.24	5.17	4.40	4.09	3.58	3.19	3.04	2.91	2.80
MeHgBr	3.94	4.58	4.05	3.83	3.46	3.15	3.03	2.91	2.81
EtHgBr	3.87	4.57	3.99	3.75	3.35	3.03	2.90	2.79	2.69
MeHgI	3.65	4.29	3.76	3.54	3.17	2.88	2.76	2.64	2.56
EtHgI	3.79	4.49	3.91	3.67	3.28	2.97	2.84	2.73	2.64
Me_2Hg	0.41	0.83	0.48	0.35	0.15	0.02	-0.02	-0.05	-0.07
Et_2Hg	0.41	0.96	0.50	0.33	0.07	-0.08	-0.13	-0.16	-0.17
Pr_2Hg	0.14	0.82	0.25	0.04	-0.26	-0.44	-0.49	-0.52	-0.52
Bu_2Hg	-0.13	0.67	0.00	-0.25	-0.60	-0.80	-0.85	-0.87	-0.88
PhHgCl	6.36	7.36	6.54	6.19	5.59	5.11	4.90	4.72	4.55
PhHgBr	5.66	6.60	5.83	5.50	4.96	4.52	4.39	4.18	4.03
PhHgI	5.35	6.26	5.51	5.20	4.68	4.27	4.10	3.95	3.82
Ph_2Hg	5.81	7.02	6.02	5.61	4.98	4.38	4.16	3.97	3.81