# SAMPL ID	$\Delta G_{hydration}$ (kcal/mol)	$\Delta G_{cyclohexane}$ (kcal/mol)	$\log D$	Stat. Unc.	Model Unc.
SAMPL5_002	-46.9 ± 0.1	-59.2 ± 0.2	2.16	0.04	1.4
SAMPL5_003	-40.8 ± 0.1	-52 ± 0.2	1.98	0.03	1.4
SAMPL5_004	-40.2 ± 0.1	-65.9 ± 0.2	4.5	0.04	1.4
SAMPL5_005	-63 ± 0.2	-69 ± 0.2	1.04	0.04	1.4
SAMPL5_006	-41.5 ± 0.1	-49.2 ± 0.2	1.34	0.03	1.4
SAMPL5_007	-40.4 ± 0.1	-66.9 ± 0.2	4.64	0.04	1.4
SAMPL5_010	-62.9 ± 0.1	-55 ± 0.2	-1.39	0.03	1.4
SAMPL5_011	-48.9 ± 0.1	-58.8 ± 0.2	1.72	0.03	1.4
SAMPL5_013	-77.2 ± 0.1	-83.5 ± 0.2	1.1	0.04	1.4
SAMPL5_015	-60.1 ± 0.1	-55.3 ± 0.1	-0.84	0.03	1.4
SAMPL5_017	-36.4 ± 0.1	-72.1 ± 0.2	6.25	0.04	1.4
SAMPL5_019	-54.8 ± 0.1	-71.2 ± 0.2	2.88	0.04	1.4
SAMPL5_020	-81.3 ± 0.1	-59.3 ± 0.2	-3.85	0.04	1.4
SAMPL5_021	-39.5 ± 0.1	-58.3 ± 0.2	3.3	0.03	1.4
SAMPL5_024	-77.1 ± 0.1	-80 ± 0.2	0.49	0.04	1.4
SAMPL5_026	-58.4 ± 0.2	-48.7 ± 0.2	-1.71	0.04	1.4
SAMPL5_027	-66 ± 0.1	-53.4 ± 0.1	-2.21	0.03	1.4
SAMPL5_033	-49.9 ± 0.1	-71.7 ± 0.2	3.82	0.04	1.4
SAMPL5_037	-72.8 ± 0.1	-46.1 ± 0.1	-4.68	0.03	1.4
SAMPL5_042	-72.7 ± 0.2	-64.9 ± 0.2	-1.36	0.05	1.4
SAMPL5_044	-61.9 ± 0.1	-76.4 ± 0.2	2.55	0.04	1.4
SAMPL5_045	-58.9 ± 0.1	-47.6 ± 0.1	-1.98	0.03	1.4
SAMPL5_046	-58.3 ± 0.1	-69.6 ± 0.2	1.97	0.04	1.4
SAMPL5_047	-48.9 ± 0.1	-67.3 ± 0.2	3.23	0.04	1.4
SAMPL5_048	-70.1 ± 0.1	-76.5 ± 0.2	1.13	0.04	1.4
SAMPL5_049	-40.5 ± 0.1	-53.1 ± 0.2	2.2	0.03	1.4
SAMPL5_050	-47.9 ± 0.2	-54.8 ± 0.1	1.2	0.04	1.4
SAMPL5_055	-46.1 ± 0.1	-43.1 ± 0.1	-0.53	0.03	1.4
SAMPL5_056	-40.5 ± 0.1	-55.9 ± 0.2	2.69	0.03	1.4
SAMPL5_058	-46 ± 0.1	-51.4 ± 0.2	0.94	0.03	1.4
SAMPL5_059	-45.8 ± 0.1	-42.1 ± 0.1	-0.66	0.03	1.4
SAMPL5_060	-74.2 ± 0.1	-53.1 ± 0.1	-3.7	0.03	1.4
SAMPL5_061	-36 ± 0.1	-46.8 ± 0.2	1.89	0.04	1.4
SAMPL5_063	-74.5 ± 0.1	-53.3 ± 0.2	-3.71	0.03	1.4
SAMPL5_065	-117.6 ± 0.2	-133.1 ± 0.3	2.72	0.06	1.4
SAMPL5_067	-38 ± 0.2	-54 ± 0.2	2.8	0.05	1.4
SAMPL5_068	-45.7 ± 0.1	-70.2 ± 0.2	4.29	0.04	1.4
SAMPL5_069	-58.8 ± 0.1	-75.3 ± 0.2	2.9	0.04	1.4
SAMPL5_070	-30.7 ± 0.1	-57.8 ± 0.2	4.74	0.04	1.4
SAMPL5_071	-54.7 ± 0.1	-59.2 ± 0.2	0.79	0.04	1.4
SAMPL5_072	-32.4 ± 0.1	-52.6 ± 0.2	3.54	0.04	1.4
SAMPL5_074	-91.6 ± 0.2	-70.2 ± 0.2	-3.76	0.04	1.4
SAMPL5_075	-43.1 ± 0.2	-58 ± 0.2	2.61	0.04	1.4
SAMPL5_080	-73.7 ± 0.1	-52.3 ± 0.1	-3.76	0.03	1.4
SAMPL5_081	-70.8 ± 0.2	-58.6 ± 0.2	-2.12	0.05	1.4
SAMPL5_082	-34.3 ± 0.2	-71.7 ± 0.2	6.56	0.05	1.4
SAMPL5_083	-142.2 ± 0.3	-149.1 ± 0.4	1.21	0.09	1.4
SAMPL5_084	-54.9 ± 0.4	-73.4 ± 0.2	3.24	0.08	1.4
SAMPL5_085	-69.1 ± 0.1	-57.5 ± 0.2	-2.03	0.04	1.4
SAMPL5_086	-58.7 ± 0.2	-76 ± 0.2	3.04	0.06	1.4
SAMPL5_088	-58.9 ± 0.1	-58.7 ± 0.2	-0.04	0.04	1.4
SAMPL5_090	-46.2 ± 0.2	-70.9 ± 0.2	4.32	0.05	1.4
SAMPL5_092	-100.6 ± 0.3	-109.3 ± 0.3	1.52	0.08	1.4

Table 1: Here are the hydration free energy and solvation free energy into cyclohexane for each molecule in the SAMPL5 challenge. The partition coefficient computed with these solvation free energies are reported as the estimate for $\log D$. Statistical uncertainty (Stat. Unc.) was reported as the propogated error fro the solvation free energy calculations. The model uncertainty (Model Unc.) was estimated from a previous study of partition coefficients in the Mobley Group.

SAMPL ID	pKa_{acidic}	pKa_{basic}	State Pen. Corr.
SAMPL5_002	11.05	4.46	0
SAMPL5_003	None	2.96	0
SAMPL5_004	13.92	6.43	-0.038
SAMPL5_005	11.49	6.37	-0.033
SAMPL5_006	10.9	5.91	-0.011
SAMPL5_007	13.97	4.57	0
SAMPL5_010	4.33	6.62	-3.337
SAMPL5_011	4.57	4.58	-3.023
SAMPL5_013	7.37	0.52	0
SAMPL5_015	4.44	5.81	-3.168
SAMPL5_017	8.93	5.76	-1.148
SAMPL5_019	13.18	5.44	-0.004
SAMPL5_020	9.74	2.65	-0.001
SAMPL5_021	None	4.92	-0.001
SAMPL5_024	11.15	5.86	-0.01
SAMPL5_026	4.23	-2.04	-3.387
SAMPL5_027	12.98	4.24	0
SAMPL5_033	12.17	2.72	0
SAMPL5_037	None	7.81	-0.571
SAMPL5_042	8.57	0.5	-0.024
SAMPL5_044	11.71	0.78	0
SAMPL5_045	11.72	1.7	0
SAMPL5_046	10.04	1.7	-0.001
SAMPL5_047	11.35	-0.83	0
SAMPL5_048	11.23	1.43	0
SAMPL5_049	10.75	-0.31	0
SAMPL5_050	-3.58	2.83	-11.902
SAMPL5_055	10.75	-0.75	0
SAMPL5_056	3.26	0.28	-4.923
SAMPL5_058	None	-1.41	0
SAMPL5_059	13.54	3.11	0
SAMPL5_060	3.75	5.93	-4.444
SAMPL5_061	None	7.72	-0.508
SAMPL5_063	13.25	9.69	-6.087
SAMPL5_065	None	8.15	-0.868
SAMPL5_067	13.32	9.25	-1.981
SAMPL5_068	None	0.83	0
SAMPL5_069	10.1	8.1	-0.842
SAMPL5_070	None	9.1	-1.817
SAMPL5_071	15.55	4.02	0
SAMPL5_072	None	8.53	-1.229
SAMPL5_074	12	3.97	0
SAMPL5_075	13.32	9.25	-1.981
SAMPL5_080	None	1.37	0
SAMPL5_081	12.67	9.25	-1.981
SAMPL5_082	None	8.37	-1.072
SAMPL5_083	7.41	6.92	-0.488
SAMPL5_084	15.03	8.72	-1.425
SAMPL5_085	7.8	2.33	-0.139
SAMPL5_086	11.73	8.87	-1.583
SAMPL5_088	14.6	5.96	-0.013
SAMPL5_090	None	4.44	0
SAMPL5_092	None	7.15	-0.194

Table 2: This table contains information for each molecule used to estimate $\log D$ from $\log P$ using either the most acidic or most basic pKa. The state penalty correction (State Pen. Corr.) is such that $\log D = \log P + correction$

SAMPL ID	$\log P$	$\log D_{pKa}$	$\log D_{statepenalty}$	$\log D_{experimental}$
SAMPL5_002	2.16	2.16	2.16	1.4
SAMPL5_003	1.98	1.98	1.98	1.9
SAMPL5_004	4.5	4.45	4.46	2.2
SAMPL5_005	1.04	1	1.01	-0.86
SAMPL5_006	1.34	1.33	1.33	-1.02
SAMPL5_007	4.64	4.64	4.64	1.4
SAMPL5_010	-1.39	-4.46	-4.73	-1.7
SAMPL5_011	1.72	-1.11	-1.3	-2.96
SAMPL5_013	1.1	0.79	1.1	-1.5
SAMPL5_015	-0.84	-3.8	-4.01	-2.2
SAMPL5_017	6.25	6.24	5.1	2.5
SAMPL5_019	2.88	2.88	2.88	1.2
SAMPL5_020	-3.85	-3.85	-3.85	1.6
SAMPL5_021	3.3	3.3	3.3	1.2
SAMPL5_024	0.49	0.48	0.48	1
SAMPL5_026	-1.71	-4.88	-5.1	-2.6
SAMPL5_027	-2.21	-2.21	-2.21	-1.87
SAMPL5_033	3.82	3.82	3.82	1.8
SAMPL5_037	-4.68	-5.23	-5.25	-1.5
SAMPL5_042	-1.36	-1.39	-1.38	-1.1
SAMPL5_044	2.55	2.55	2.55	1
SAMPL5_045	-1.98	-1.98	-1.98	-2.1
SAMPL5_046	1.97	1.97	1.97	0.2
SAMPL5_047	3.23	3.23	3.23	-0.4
SAMPL5_048	1.13	1.13	1.13	0.9
SAMPL5_049	2.2	2.2	2.2	1.3
SAMPL5_050	1.2	-9.78	-10.7	-3.2
SAMPL5_055	-0.53	-0.53	-0.53	-1.5
SAMPL5_056	2.69	-1.45	-2.23	-2.5
SAMPL5_058	0.94	0.94	0.94	0.8
SAMPL5_059	-0.66	-0.66	-0.66	-1.3
SAMPL5_060	-3.7	-7.35	-8.14	-3.9
SAMPL5_061	1.89	1.4	1.39	-1.45
SAMPL5_063	-3.71	-6.01	-9.8	-3
SAMPL5_065	2.72	1.9	1.85	0.7
SAMPL5_067	2.8	0.94	0.82	-1.3
SAMPL5_068	4.29	4.29	4.29	1.4
SAMPL5_069	2.9	2.12	2.05	-1.3
SAMPL5_070	4.74	3.03	2.92	1.6
SAMPL5_071	0.79	0.79	0.79	-0.1
SAMPL5_072	3.54	2.38	2.31	0.6
SAMPL5_074	-3.76	-3.76	-3.76	-1.9
SAMPL5_075	2.61	0.75	0.63	-2.8
SAMPL5_080	-3.76	-3.76	-3.76	-2.2
SAMPL5_081	-2.12	-3.98	-4.1	-2.2
SAMPL5_082	6.56	5.55	5.49	2.5
SAMPL5_083	1.21	0.91	0.72	-1.9
SAMPL5_084	3.24	1.89	1.81	0
SAMPL5_085	-2.03	-2.18	-2.17	-2.2
SAMPL5_086	3.04	1.56	1.46	0.7
SAMPL5_088	-0.04	-0.06	-0.05	-1.9
SAMPL5_090	4.32	4.32	4.32	0.8
SAMPL5_092	1.52	1.33	1.33	-0.4

Table 3: Here are results for $\log P$ computed from calculated solvation free energies, then corrected to $\log D$ by pKa ($\log D_{pKa}$) or by state penalty ($\log D_{statepenalty}$), compared with the experimentally reported values for $\log D$