Supporting Material for "Automated parametrization of the coarse-grained Martini force field for small organic molecules"

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Fig. S1 shows the water/octanol free energy of partitioning for the 354 neutral compounds presented in Figure 5 of the main text—used to compute the set of hydration free energies—comparing between CG simulations and predicted data from ALOGPS. The data shows high correlation ($R^2 = 0.91$) and a mean-absolute error of 0.70 kcal/mol, on par with the correlation study presented in Figure 4 of the main text on the 607 neutral compounds.

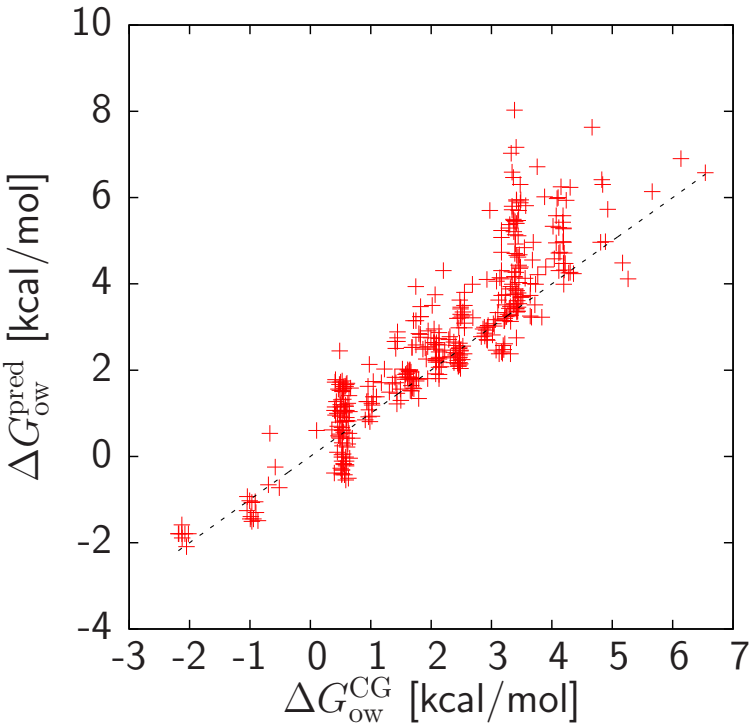

FIG. S1: Water/octanol free energy of partitioning for the 354 neutral compounds presented in Figure 5 of the main text: comparison between CG simulations ($\Delta G_{\rm ow}^{\rm CG}$) and predicted data from ALOGPS ($\Delta G_{\rm ow}^{\rm pred}$). Correlation coefficient: $R^2 = 0.91$; MAE: 0.70 kcal/mol. CG error bars: ≈ 0.1 kcal/mol, not shown for clarity.

Tab. S1 and Tab. S3 provide the reference and coarse-grained (CG) free energy of water/octanol partitioning and hydration, respectively, of all molecules used in this study.

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TABLE S1: SMILES string, CAS registry number, and experimental and CG water/octanol free energy of partitioning for all 653 neutral compounds used in this work. Units are in kcal/mol.

#	SMILES	CAS	$\Delta G_{\mathrm{ow}}^{\mathrm{exp}}$	$\Delta G_{\mathrm{ow}}^{\mathrm{CG}}$
1	BrC(F)(F)F	75-63-8	2.54	2.46
2	FC(F)(F)F	75-73-0	1.61	2.45
3	BrC(Br)(Br)CO	75-80-9	2.87	2.94
4	C=CCC=C	591-93-5	3.39	3.31
5	C=CCl	75-01-4	2.08	1.62
6	CC=CC=C	1574-41-0	3.28	3.38
7	CC=CC=C	2004-70-8	3.34	3.38
8	C1C(Br)C(Br)CN(N=O)C1	57541-73-8	1.68	2.36
9	n1c(N)nc(Cl)nc1NCC	1007-28-9	1.57	0.34
10	ClC(Cl)(Cl)C(O)NC(=O)OCC	541-79-7	2.52	0.74
11	FCC(F)Cl	338-64-7	2.21	1.33
12	CC1=NNC(C)=C1	67-51-6	1.38	0.94
13	CC1=NON=C1CC	17647-69-7	1.61	2.35
14	CC(F)(Cl)Cl	1717-00-6	2.53	2.97
15	C1=C(C)N=C(N=C(N)N)S1	7120-01-6	1.70	-1.22
16	C=CC(=O)OCC	140-88-5	1.80	1.96
17	ClC(Cl)(Cl)C	71-55-6	3.40	3.38
18	ClCC(Cl)Cl	79-00-5	2.58	2.60
19	FC(F)(F)CC(C)CO	114525-06-3	1.90	1.45
20	FC(F)(F)C(C)CCO	95853-68-2	1.87	1.56
21	FC(F)(F)CCCCO	352-61-4	1.57	1.40
22	CC1NCC=C1	122970-63-2	2.56	0.53
23	C1C(O)CC(C(=O)O)N1	51-35-4	-4.34	-3.08
24	CC(=O)NC(C)C(=O)O	97-69-8	-4.02	-1.12
25	CCC(N=C=S)C	4426-79-3	3.84	4.01
26	S=C=NCC(C)C	591-82-2	3.86	3.66
27	CCCCN=C=S	592-82-5	3.99	4.08
28	C1CCCC1	287-92-3	4.10	4.62
29	C=CCCC	109-67-1	3.83	3.40
30	CC=C(C)C	513-35-9	3.65	3.45
31	NC(=O)C(C)NC(=O)C	15962-47-7	-2.08	-2.77
32	CC(=O)NCC(=O)NC	7606-79-3	-2.13	-1.72
33	NC(=O)CCC(N)C(=O)O	56-85-9	-4.31	-3.17
34	OCC(C(=O)N)NC(=O)C	23361-38-8	-2.56	-3.77
35	CC1CCCO1	96-47-9	1.71	0.57
36	CCCCC(=O)O	109-52-4	1.90	1.71
37	CCC(C)C(=O)O	116-53-0	1.61	2.01
38	OC(=O)C(C)(C)C	75-98-9	2.01	2.09
39	OC(=O)CC(C)C	503-74-2	1.59	2.42
40	CCCC(=O)OC	623-42-7	1.76	2.08

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
41	CC(=O)OC(C)C	108-21-4	1.40	0.98
42	CCOC(=O)OCC	105-58-8	1.65	0.51
43	C1(CO)C(O)C(O)C(O)C(O)O1	50-69-1	-3.17	-5.25
44	C1C(O)C(O)C(O)C(O)C(O)O1	147-81-9	-4.13	-5.10
45	CS(=O)(=O)OCC(O)C1CO1	30031-63-1	-1.61	-1.50
46	CCCCCBr	110-53-2	4.61	4.12
47	CCC(C)(C)Cl	594-36-5	3.45	3.46
48	CCCCCCl	543-59-9	4.25	4.32
49	CCCCCF	592-50-7	3.19	3.38
50	CCCCCI	628-17-1	4.95	4.68
51	CCCC(N)C(=O)O	6600-40-4	-2.54	-2.24
52	CC(C)C(N)C(=O)O	72-18-4	-3.09	-2.16
53	NCCCCC(=O)O	660-88-8	-3.60	-2.20
54	CCCC(N)C(=O)O	760-78-1	-2.89	-2.24
55	O1C(N)=NN=C1	3775-60-8	-1.97	-1.81
56	CCNC(CO)C(=O)O	83293-50-9	-3.43	-2.72
57	CS(=O)(=O)CCC(N)C(=O)O	7314-32-1	-4.24	-3.17
58	CCCCC	109-66-0	4.64	3.43
59	CC(C)(C)C	463-82-1	4.25	3.38
60	CCCCCO	71-41-0	2.06	1.58
61	CC(C)CCO	123-51-3	1.75	2.13
62	CC(C)(C)CO	75-84-3	1.79	1.59
63	C=C	74-85-1	1.55	0.88
64	CCC(O)CC	584-02-1	1.65	1.60
65	COCCCC	628-28-4	2.27	2.45
66	CNCCCC	110-68-9	1.82	1.66
67	CCCCCN	110-58-7	2.04	1.67
68	S=P(C)(OCC)OCC	6996-81-2	2.85	1.24
69	BrCCBr	106-93-4	2.68	1.83
70	CC[Pb](C)(C)C	1762-26-1	5.30	2.33
71	CCC[Si](C)C	18143-31-2	4.40	3.86
72	c1(Br)c(Br)c(Br)c(Br)c(Br)c1Br	87-82-1	8.30	7.80
73	c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	608-93-5	7.07	7.38
74	c1(O)c(F)c(F)c(F)c(F)c1F	771-61-9	4.42	4.33
75	CC(Cl)Cl	75-34-3	2.45	2.43
76	c1(Br)c(Br)cc(Br)c(Br)c1	636-28-2	7.01	7.02
77	c1(Cl)c(Cl)cc(Cl)c(Cl)c1	95-94-3	6.33	7.11
78	ClCCCl	107-06-2	2.02	1.85
79	Fc1cc(F)c(F)cc1F	327-54-8	3.34	4.86
80	Brc1cccc(Cl)c1Cl	56961-77-4	6.30	6.19
81	Clc1cccc(Cl)c1Br	19393-92-1	5.70	6.24
82	c1(Br)cc(Br)cc(Br)c1	626-39-1	6.17	6.51
83	c1(Br)c(O)c(Br)cc(Br)c1	118-79-6	5.58	4.05

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
84	S=C=S	75-15-0	2.65	2.89
85	FCC(=O)N	640-19-7	-1.44	-0.96
86	C1=Cc2ncnc(Cl)c2S1	16269-66-2	2.45	3.43
87	Clc1cccc(Cl)c1F	2268-05-5	4.62	5.75
88	Clc1cc(Cl)ccc1F	1435-48-9	4.62	5.96
89	OC(=O)c1cc(Cl)nc(Cl)c1	5398-44-7	3.55	2.12
90	c1(Cl)cc(Cl)cc(Cl)c1	108-70-3	5.67	6.58
91	c1c(Cl)c(Cl)c(Cl)cc1	87-61-6	5.54	6.24
92	c1c(O)c(Cl)c(Cl)c(Cl)c1	15950-66-0	4.94	5.24
93	c1(O)cc(Cl)c(Cl)c(Cl)c1	609-19-8	5.48	5.31
94	Nc1c(Cl)c(Cl)cc(Cl)c1Cl	3481-20-7	5.61	5.88
95	ClC(Cl)(Cl)c1nc(C(Cl)(Cl)Cl)nc(SC)n1	3599-76-6	6.04	2.30
96	c1c(F)c(F)cc(F)c1	367-23-7	3.30	4.32
97	Oc1c(I)cc(I)cc1I	609-23-4	6.15	5.44
98	ICCI	624-73-7	3.70	3.04
99	c1c(Br)ccc(Br)c1	106-37-6	5.18	4.75
100	c1c(Br)cc(Br)cc1	108-36-1	5.13	5.85
101	c1c(O)c(Br)cc(Br)c1	615-58-7	4.45	4.43
102	Brc1cccc(Br)c1O	608-33-3	4.60	3.40
103	Brc1c(Br)cccc1O	57383-80-9	4.61	4.40
104	Ic1ccc(Cl)cc1	637-87-6	5.63	5.95
105	C1(=NCl)C=CC(=O)C=C1	637-61-6	1.72	1.18
106	c1cc(C(=O)O)nc(Cl)c1	4684-94-0	2.05	1.85
107	N1c2ccc(Cl)cc2N=N1	94-97-3	2.97	3.03
108	c1c(Cl)c(Cl)ccc1	95-50-1	4.62	5.81
109	c1c(Cl)ccc(Cl)c1	106-46-7	4.72	5.53
110	c1c(Cl)cc(Cl)cc1	541-73-1	4.81	5.77
111	c1(Cl)cc(O)cc(Cl)c1	591-35-5	4.94	4.86
112	c1c(Cl)cc(O)c(Cl)c1	583-78-8	4.29	4.61
113	c1c(O)cc(Cl)c(Cl)c1	95-77-2	4.55	4.11
114	c1c(O)c(Cl)cc(Cl)c1	120-83-2	4.34	4.66
115	c1c(Cl)c(O)c(Cl)cc1	87-65-0	3.61	3.43
116	c1(N)c(Cl)cc(Cl)c(Cl)c1	636-30-6	4.72	5.39
117	c1(N)cc(Cl)c(Cl)c(Cl)c1	634-91-3	4.54	5.42
118	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1Cl	59229-56-0	5.63	4.37
119	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1Cl	57722-17-5	5.95	4.37
120	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1Cl	57722-15-3	5.89	4.37
121	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1Cl	57722-16-4	5.94	4.37
122	Fc1cc(F)ccc1	372-18-9	3.32	4.17
123	BrC(Cl)Cl	75-27-4	2.74	2.59
124	Fc1ccccc1F	367-11-3	3.24	4.22
125	Fc1cccc(F)c1O	28177-48-2	2.80	4.07
126	Nc1c(F)cc(F)cc1F	363-81-5	2.48	3.10

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
127	C1=CC2=NON=C2C=C1	273-09-6	2.31	3.47
128	N1=C2C=CC=CC2=NS1	273-13-2	2.75	2.20
129	c1ccccc1Br	108-86-1	4.09	3.64
130	c1c(Br)cc(O)cc1	591-20-8	3.55	3.93
131	c1c(Br)c(O)ccc1	95-56-7	3.19	2.72
132	COC(=O)C1=CC=C(Br)O1	2527-99-3	2.52	1.83
133	c1ccccc1Cl	108-90-7	3.88	5.05
134	c1c(N)cc(Cl)c(F)c1	367-21-5	2.74	4.00
135	Nc1ccc(F)cc1Cl	2106-02-7	2.79	3.86
136	Cl[Hg]c1ccccc1	100-56-1	2.43	3.06
137	c1cc([Hg]Cl)c(O)cc1	90-03-9	2.06	2.04
138	c1c(Cl)ccc(O)c1	106-48-9	3.27	4.06
139	c1c(Cl)cc(O)cc1	108-43-0	3.42	3.86
140	OCC(=O)O	79-14-1	-1.52	-0.92
141	c1c(O)c(Cl)cc(O)c1	615-67-8	1.91	3.21
142	c1c(N)c(Cl)c(Cl)cc1	608-27-5	3.86	4.56
143	c1c(Cl)c(N)c(Cl)cc1	608-31-1	3.77	4.64
144	c1c(N)c(Cl)cc(Cl)c1	554-00-7	3.80	4.83
145	c1(Cl)cc(N)cc(Cl)c1	626-43-7	3.97	4.84
146	c1c(Cl)cc(N)c(Cl)c1	95-82-9	3.76	4.47
147	c1c(N)cc(Cl)c(Cl)c1	95-76-1	3.66	4.65
148	CCBr	74-96-4	2.20	2.45
149	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1	51795-30-3	5.20	3.79
150	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1	54083-25-9	5.26	3.79
151	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1	54083-24-8	4.92	3.79
152	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1	643-15-2	4.94	3.79
153	C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)=C1	319-94-8	5.40	3.79
154	c1ccccc1F	462-06-6	3.10	4.08
155	c1c(F)ccc(O)c1	371-41-5	2.42	3.24
156	c1c(F)cc(O)cc1	372-20-3	2.64	3.20
157	c1cc(F)c(O)cc1	367-12-4	2.28	4.18
158	ClC(Br)Br	124-48-1	2.95	2.96
159	CCCl	75-00-3	1.95	1.78
160	c1c(N)c(F)cc(F)c1	367-25-9	2.12	3.15
161	Nc1c(F)cccc1F	5509-65-9	2.20	3.13
162	c1cc(S(F)(F)(F)(F)F)ccc1	2557-81-5	4.60	2.87
163	c1ccccc1I	591-50-4	4.45	4.19
164	c1c(I)cc(O)cc1	626-02-8	4.01	3.30
165	c1c(I)ccc(O)c1	540-38-5	3.97	4.35
166	c1c(I)c(O)ccc1	533-58-4	3.62	3.32
167	c1ccc(N=O)cc1	586-96-9	2.74	3.60
168	CCI	75-03-6	2.74	3.21
169	N1=Nc2ccccc2N1	95-14-7	1.97	1.17

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
170	CC(=O)N	60-35-5	-1.72	-0.87
171	c1ccccc1	71-43-2	2.91	4.17
172	BrC1C(F)C(Cl)C(Cl)C(Cl)C1Cl	55265-51-5	4.49	4.31
173	C1(Br)C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	36635-03-7	5.21	8.16
174	C1(Br)C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	36635-02-6	5.11	8.16
175	c1c(Br)c(N)ccc1	615-36-1	2.89	2.57
176	c1c(Br)cc(N)cc1	591-19-5	3.00	4.05
177	c1c(Cl)c(N)ccc1	95-51-2	2.60	3.92
178	c1c(Cl)ccc(N)c1	106-47-8	2.50	4.06
179	c1c(Cl)cc(N)cc1	108-42-9	2.57	3.90
180	Oc1ccc(Cl)cc1N	95-85-2	2.48	3.07
181	C1(Cl)C(Cl)C(Cl)C(Cl)C=C1	41992-55-6	4.65	3.67
182	C1(Cl)c(Cl)C(Cl)C=C(Cl)c1	89674-85-1	5.09	4.50
183	C1(Cl)C(Cl)C(Cl)C=C(Cl)C1	89674-87-3	4.99	4.50
184	C1(Cl)C(Cl)C(Cl)C=C(Cl)C1	89674-88-4	4.81	4.50
185	C1(Cl)C(Cl)C(Cl)C(Cl)C=C1	1782-00-9	4.21	3.67
186	C1(Cl)C(Cl)C(Cl)C(Cl)C=C1	33875-95-5	4.31	3.67
187	CC(=O)NO	546-88-3	-2.17	-2.15
188	C1(Cl)C(Cl)C(Cl)C(Cl)C=C1	28810-38-0	5.11	3.67
189	C1(Cl)C(Cl)C(Cl)C(Cl)C=C1	319-81-3	4.21	3.67
190	C1(F)C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	56086-55-6	4.36	3.98
191	C1(I)C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	33489-28-0	5.41	6.00
192	C1(I)C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	33489-27-9	5.54	6.00
193	ClC(F)F	75-45-6	1.48	1.61
194	c1c(F)c(N)ccc1	348-54-9	1.72	3.14
195	c1c(F)cc(N)cc1	372-19-0	1.78	3.00
196	c1c(F)ccc(N)c1	371-40-4	1.57	3.35
197	c1c(I)cc(N)cc1	626-01-7	3.97	3.27
198	c1c(I)c(N)ccc1	615-43-0	3.17	3.29
199	N1=C(N)NN=C1N	1455-77-2	-2.20	-1.82
200	CC	74-84-0	2.48	1.65
201	N1C(C(=O)NC(=O)N2C)=C2NC1=O	605-99-2	-1.48	-4.28
202	CN1C(C(=O)NC(=O)N2)=C2NC1=O	612-37-3	-1.61	-4.61
203	c1ccccc1O	108-95-2	2.05	3.29
204	C1=CSC(C(=O)C)=C1	88-15-3	1.71	3.34
205	C1=CSC=C1C(=O)C	1468-83-3	1.70	3.10
206	C1=CSC=C1C(=O)OC	22913-26-4	2.41	2.08
207	COC(=O)C1=CC=CS1	5380-42-7	2.50	2.02
208	O=C1SSC(C(=O)C)=C1C	620957-94-0	2.16	1.43
209	C1=COC(C(=O)OC)=C1	611-13-2	1.37	0.70
210	O1C=CC(C(=O)OC)=C1	13129-23-2	1.75	0.85
211	O1C(=O)C(=O)C(=O)C1C(O)CO	36355-38-1	-2.41	-2.71
212	c1cc(S)ccc1	108-98-5	3.45	5.15

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
213	S1SC=2CCCC2C1=S	14085-33-7	3.46	5.54
214	c1c(C)nc(Cl)c(C)n1	95-89-6	2.05	0.13
215	FC(Cl)Cl	75-43-4	2.12	1.60
216	NC(=O)NC	598-50-5	-1.91	-2.10
217	Nc1ccc(Cl)cc1N	95-83-0	1.75	2.96
218	C1C(Cl)C(Cl)C(Cl)C=C1	56994-25-3	3.88	4.48
219	C=C(C)C(=O)OCC(F)(F)F	352-87-4	2.13	2.32
220	CNC(=S)NCC(F)(F)C(F)(F)C(F)(F)F	105412-23-5	2.72	2.12
221	c1c(C)ccnc1	108-89-4	1.67	2.25
222	c1c(C)cncc1	108-99-6	1.64	2.14
223	CC(=O)NN	1068-57-1	-2.16	-2.14
224	c1c(C)nccc1	109-06-8	1.52	2.03
225	c1c(OC)nccc1	1628-89-3	1.86	1.72
226	C1(=O)C=CN(C)C=C1	695-19-2	-1.67	0.61
227	c1c(OC)ccnc1	620-08-6	1.37	1.71
228	C1=CSC=C1C(=NO)C	59445-83-9	2.48	3.04
229	C1=CSC(NC(=O)C)=C1	13053-81-1	1.50	2.36
230	C1=CNC(C(=O)OC)=C1	1193-62-0	1.98	0.22
231	S1C=CC=C1C(N)C(=O)O	21124-40-3	-2.80	1.10
232	c1nc(SC)ccc1	18438-38-5	2.34	2.62
233	c1c(N)c(S)ccc1	137-07-5	1.95	3.97
234	Nc1ccc(S)cc1	1193-02-8	1.79	4.01
235	CS(=O)C	67-68-5	-1.85	-0.88
236	C1C=CC=CC1	592-57-4	3.38	3.27
237	C1C=CCC=C1	628-41-1	3.15	3.29
238	OCCO	107-21-1	-1.86	-2.02
239	S1C(CCCl)=C(C)N=C1	533-45-9	2.90	2.65
240	n1cc(Cl)nc(N(C)C)c1	61655-72-9	2.67	1.63
241	ClC(Cl)Cl	67-66-3	2.69	2.46
242	CS(=O)(=O)C	67-71-0	-1.83	-0.90
243	C1(Cl)C(Cl)CC(Cl)C(Cl)C1	60067-92-7	3.86	8.25
244	c1c(NN)cccc1	100-63-0	1.71	3.30
245	c1c(NC)nccc1	4597-87-9	1.50	1.68
246	CSC	75-18-3	1.44	0.93
247	c1c(N)ncc(C)c1	1603-41-4	1.40	1.83
248	CSSC	624-92-0	2.42	1.68
249	n1cc(C)nc(OC)c1	2882-21-5	1.76	1.50
250	c1nc(C)c(OC)nc1	2847-30-5	1.70	-1.81
251	n1cc(OC)nc(OC)c1	4774-15-6	2.16	1.39
252	c1c(OC)ncc(OC)n1	117856-61-8	1.56	1.31
253	c1nc(C)c(SC)nc1	2882-20-4	2.48	1.18
254	c1c(SC)nnc(SC)c1	37813-54-0	2.53	0.45
255	C1=COC(CC)=C1	3208-16-0	3.28	3.30

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
256	NCCO	141-43-5	-1.79	-2.18
257	CC1=CC=C(C)O1	625-86-5	3.06	3.02
258	CCCC1=CSSC1=O	164584-60-5	3.25	3.82
259	CCCC1=CC(=O)SS1	164584-62-7	3.06	3.80
260	CC=CC=CC(=O)O	110-44-1	1.82	2.49
261	O1C(=O)C(O)=C(O)C1C(O)CO	50-81-7	-2.24	-2.98
262	OC(=O)CC(O)(C(=O)O)CC(=O)O	77-92-9	-2.15	-2.06
263	CN(O)C	5725-96-2	-1.57	-0.91
264	C1=CSC(CC)=C1	872-55-9	3.92	3.98
265	C1=CSC=C1CC	1795-01-3	3.86	3.88
266	CCCC1=CC(=S)SS1	146252-77-9	3.87	4.23
267	CCCC1=CSSC1=S	38696-40-1	4.35	4.95
268	CCC1=C(C)SSC1=S	55486-68-5	4.02	4.08
269	CCC1=C(C)C(=S)SS1	6125-90-2	4.03	4.76
270	CNC(=O)NN	17696-95-6	-3.01	-2.24
271	CC1=CC=C(C)N1	625-84-3	2.01	1.32
272	CCC1=CC=CN1	1551-06-0	2.17	2.01
273	n1c(N(C)C)nccc1	5621-02-3	1.46	-0.50
274	N1=CNC=C1CC(N)C(=O)O	71-00-1	-3.45	-0.38
275	C1CCC=CC1	110-83-8	3.91	5.30
276	CC=CC=CC	5194-50-3	3.83	3.38
277	NCCN	107-15-3	-2.79	-2.28
278	CC=CC=CC	5194-51-4	4.12	3.38
279	CC=CC=CC	6108-61-8	4.32	3.38
280	C=CCC=CC	592-45-0	4.32	3.38
281	C1C(Cl)C(Cl)CCC1	10498-35-8	4.35	5.90
282	C1C(Cl)C(Cl)CCC1	822-86-6	4.39	5.90
283	N1C=CN=C1CCC	50995-95-4	1.78	1.08
284	N1N=CC(OCCC)=C1	88095-60-7	1.94	2.36
285	N1N=CC(OC(C)C)=C1	14884-03-8	1.55	2.48
286	CC1=NON=C1CCC	77580-78-0	2.34	3.48
287	NC(=O)CN1CCCC1=O	7491-74-9	-2.10	-1.78
288	NC(=O)C(NC(=O)C)CC(=O)O	4033-40-3	-3.55	-2.24
289	CC(=O)CCC=C	109-49-9	1.40	1.79
290	C=C(C)C(=O)OCC	97-63-2	1.78	2.93
291	FC(F)(F)C(F)=C(F)F	116-15-4	2.57	2.12
292	OC(=O)C1CCCC1	3400-45-1	2.08	4.72
293	BrC(Br)(Br)Br	558-13-4	4.68	3.38
294	FC(F)(F)C(=O)C(F)(F)F	10057-27-9	2.00	1.38
295	C1OC1C(O)C(O)C2OC2	23261-20-3	-1.76	-2.75
296	C1(C(=O)O)C(O)C(O)C(O)C(O)O1	6556-12-3	-3.51	-4.29
297	BrC1CCCCC1	108-85-0	4.38	6.61
298	NC(=O)NC(=O)C(Br)C(C)C	496-67-3	1.56	0.15

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
299	NC(=O)NC(=O)C(Cl)C(C)C	61345-66-2	1.37	0.08
300	O1C(O)C(F)C(O)C(O)C1CO	62182-10-9	-2.60	-3.46
301	FC(F)(F)CCCCCO	65611-47-4	2.24	1.45
302	FC(F)(F)CC(C)CCO	107103-97-9	2.20	1.46
303	FC(F)(F)CCC(O)CC	107103-96-8	2.32	2.60
304	C=CCNCC=C	124-02-7	1.52	1.29
305	C1CC(N)(C(=O)O)CC1	52-52-8	-3.53	-2.15
306	N1C(Br)=NC(Br)=C1Br	2034-22-2	2.68	1.86
307	NC(=O)CC(NC(=O)C)C(=O)N	84652-30-2	-3.30	-4.38
308	N1C(Cl)=C(Cl)N=C1Cl	7682-38-4	2.53	1.83
309	NCC(=O)NCC(=O)NCC(=O)O	556-33-2	-3.66	-5.10
310	C1CC(C)CC1	96-37-7	4.61	5.09
311	C=CCCCC	592-41-6	4.65	3.42
312	C1CCCCC1	110-82-7	4.70	8.99
313	FC(F)(F)C(F)C(F)(F)F	431-89-0	2.89	2.14
314	ClCC(C)OC(C)CCl	108-60-1	3.39	2.50
315	CCN(CC)CC(F)(F)F	37174-09-7	2.57	2.39
316	N1CC(I)=NC(I)=C1I	1746-25-4	3.80	2.36
317	CC(=O)NC(C)C(=O)NC	22715-68-0	-1.65	-2.11
318	CC(O)C(C(=O)N)NC(=O)C	60828-33-3	-2.15	-3.75
319	BrC(Cl)C(F)(F)C1N=N1	427897-90-3	2.60	1.24
320	C1CCC(O)CC1	108-93-0	1.68	1.85
321	C1C(C)OC(C)C1	2144-41-4	1.67	2.62
322	C1C(C)OC(C)C1	2390-94-5	1.83	2.62
323	CC(=O)CC(C)C	108-10-1	1.79	2.20
324	CC(=O)CCCC	591-78-6	1.89	2.04
325	CCCCCC=O	66-25-1	2.43	3.75
326	CCCCC1OC1	1436-34-6	2.67	3.39
327	CC(=O)C(C)(C)C	75-97-8	1.64	2.37
328	CC(=O)OCCCC	123-86-4	2.43	3.19
329	FC(F)(F)C(Cl)OC(F)F	26675-46-7	2.82	1.95
330	CCC(CC)C(=O)O	88-09-5	2.30	2.40
331	CCCC(C)C(=O)O	97-61-0	2.46	3.22
332	CCCCCC(=O)O	142-62-1	2.63	3.24
333	CC(=O)OC(C)CC	105-46-4	2.35	3.65
334	CC(=O)OC(C)(C)C	540-88-5	2.41	3.20
335	COC(=O)CC(C)C	556-24-1	2.49	2.17
336	COC(=O)C(C)(C)C	598-98-1	2.50	2.15
337	CCCCC(=O)OC	624-24-8	2.68	3.27
338	FC(Cl)C(F)(F)OC(F)F	13838-16-9	2.87	1.94
339	CC(=O)OCC(C)C	110-19-0	2.43	3.41
340	CCC(=O)OCCC	106-36-5	2.34	3.25
341	CCC(=O)OC(C)C	637-78-5	2.15	3.32

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
342	CCCC(=O)OCC	105-54-4	2.34	3.22
343	CC(C)C(=O)OCC	97-62-1	2.12	3.20
344	C1(O)C(O)C(O)C(O)C(CO)O1	50-99-7	-4.43	-5.37
345	OCC(O)C(O)C(O)C(O)C=O	921-60-8	-4.50	-4.85
346	CCCCCCBr	111-25-1	5.20	4.87
347	CCCCCCCl	544-10-5	5.00	4.74
348	CCCCCCI	638-45-9	5.69	5.38
349	C=CCNCCC	5666-21-7	1.82	2.17
350	C1CCN(C)CC1	626-67-5	1.78	1.95
351	C1CCCCC1N	108-91-8	2.04	2.00
352	NC(=O)OCCCCC	638-42-6	1.85	2.14
353	CN(C)C(=O)OC(C)C	38580-89-1	1.89	1.61
354	CCCCC(N)C(=O)O	327-57-1	-2.09	-2.26
355	CC(C)CC(N)C(=O)O	61-90-5	-2.38	-2.23
356	CCC(C)C(N)C(=O)O	73-32-5	-2.41	-2.24
357	NCCCCCC(=O)O	60-32-2	-4.03	-2.20
358	CCCCC(N)C(=O)O	616-06-8	-2.10	-2.26
359	CCCCCC	110-54-3	5.33	3.41
360	CC(C)C(C)C	79-29-8	4.68	3.39
361	CCC(C)(C)C	75-83-2	5.22	3.37
362	CCC(C)CC	96-14-0	4.92	3.37
363	CC(C)(C)CN(C)N=O	31820-22-1	2.90	2.07
364	N=C(N)NCCCC(N)C(=O)O	74-79-3	-5.74	-3.29
365	CCCOCCC	111-43-3	2.78	3.04
366	CC(C)OC(C)C	108-20-3	2.08	2.40
367	CCOCCCC	628-81-9	2.78	2.92
368	CCCCCCO	111-27-3	2.78	3.23
369	CC(C)(C)C(C)O	464-07-3	2.02	2.14
370	CCC(O)CCC	623-37-0	2.26	2.49
371	CC(O)CCCC	626-93-7	2.41	2.58
372	CCCC(C)(O)C	590-36-3	2.09	2.46
373	CC(C)C(O)(C)C	594-60-5	2.02	2.46
374	CCC(CC)CO	97-95-0	2.43	2.91
375	S=C1C=CSS1	534-25-8	2.16	1.85
376	CC(C)CC(O)C	108-11-2	2.28	3.19
377	BrCCl	74-97-5	1.93	1.66
378	CC(C)SC(C)C	625-80-9	3.88	5.13
379	CCCSCCC	111-47-7	4.05	5.15
380	CCCNCCC	142-84-7	2.28	2.47
381	CCCCN(C)C	927-62-8	2.32	3.13
382	CCN(CC)CC	121-44-8	1.98	2.43
383	CCCCCCN	111-26-2	2.82	3.26
384	ClC(Cl)(Cl)C(=O)OC	598-99-2	2.78	1.83

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
385	OCCN(CCO)CCO	102-71-6	-1.37	-2.83
386	N=C(N)NC(=N)NCCCC	692-13-7	-1.64	-1.84
387	CC[Pb](CC)(C)C	1762-27-2	5.52	2.11
388	CCC[Si](C)(C)C	3510-70-1	5.25	4.49
389	CCCC[Si](C)(C)C	1001-52-1	4.88	4.08
390	N1C=C(I)C=N1	3469-69-0	2.32	2.24
391	Brc1c(Cl)c(Cl)c(Cl)c(Br)c1OC	174913-68-9	7.59	7.06
392	Brc1c(Br)c(Br)c(Br)c(Br)c1OC	1825-26-9	7.43	7.49
393	C1(C(F)(F)F)=Nc2ncc(Cl)cc2N1	13577-71-4	3.36	2.88
394	COc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	1825-21-4	7.45	7.78
395	c1(F)c(F)c(F)c(S(=O)(=O)C)c(F)c1F	651-85-4	1.52	1.91
396	C1(C(F)(F)F)(C(F)(F)F)NC(C(F)(F)F)(C(F)(F)F)N=C1N	23757-42-8	4.58	2.02
397	BrCBr	74-95-3	2.57	1.56
398	Brc1cc(Cl)c(Cl)c(Cl)c1OC	174913-31-6	6.35	7.26
399	Brc1c(Cl)c(Cl)c(Cl)cc1OC	174913-24-7	6.80	6.73
400	OC(=O)c1ccc(Br)cc1F	112704-79-7	3.65	4.69
401	OC(=O)c1c(Br)cccc1Br	601-84-3	4.90	4.61
402	Brc1cc(Br)c(Cl)c(Br)c1OC	174913-78-1	7.23	7.21
403	OC(=O)c1c(Cl)cccc1F	434-75-3	2.89	4.15
404	O=C1Nc2cc(Cl)ccc2O1	95-25-0	2.89	2.95
405	c1c(Cl)c(Cl)c(OC)c(Cl)c1Cl	6936-40-9	6.40	6.74
406	c1(O)c(OC)c(Cl)c(Cl)c(Cl)c1Cl	2539-17-5	6.29	3.71
407	C1(C(F)(F)F)=Nc2ncccc2N1	13797-63-2	1.89	2.65
408	OC(=O)c1cc(I)c(O)c(I)c1	618-76-8	5.06	3.68
409	S1Sc2ccccc2C1=S	3354-42-5	4.88	4.35
410	ClCCl	75-09-2	1.71	1.64
411	N1C=NC(=O)NC1=O	71-33-0	-2.56	-5.43
412	Clc1cc(OC)cc(Cl)c1Br	174913-20-3	6.00	6.19
413	c1c(Br)c(Cl)c(Cl)c(OC)c1	109803-52-3	6.11	5.81
414	Clc1cc(Cl)cc(Br)c1OC	60633-26-3	5.47	6.55
415	c1c(Br)cc(C(=O)O)cc1	585-76-2	3.76	2.98
416	c1c(Br)ccc(C(=O)O)c1	586-76-5	3.83	4.74
417	c1c(Br)c(C(=O)O)ccc1	88-65-3	2.97	2.80
418	O=C1C(Br)=CC(=O)C=C1C	6293-55-6	1.65	1.85
419	O=Cc1cc(Br)cc(O)c1	199177-26-9	3.42	3.01
420	Brc1cc(Cl)cc(Br)c1OC	174913-44-1	5.92	6.57
421	c1(Br)cc(Br)c(OC)c(Br)c1	607-99-8	6.13	6.73
422	FC(F)(F)c1cc(N)c(Cl)cc1	121-50-6	4.18	4.50
423	O1c2ccc(Cl)cc2N=C1N	61-80-3	3.36	3.03
424	c1c(Cl)c(C=O)ccc1	89-98-5	3.19	3.53
425	O=Cc1cc(Cl)ccc1	587-04-2	3.09	3.76
426	c1c(Cl)c(C(=O)O)ccc1	118-91-2	2.72	4.08
427	c1c(Cl)cc(C(=O)O)cc1	535-80-8	3.55	4.83

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
428	c1c(O)c(C(=O)O)cc(Cl)c1	321-14-2	4.23	2.76
429	C=C=C	463-49-0	1.98	2.36
430	c1c(Cl)cc(Cl)c(CCl)c1	94-99-5	5.22	6.23
431	c1c(Cl)c(Cl)c(OC)cc1Cl	54135-81-8	5.37	6.35
432	c1c(Cl)c(Cl)c(Cl)cc1OC	54135-82-9	5.77	6.11
433	c1c(Cl)c(OC)c(Cl)cc1Cl	87-40-1	5.62	6.64
434	c1c(F)cc(C(=O)O)cc1	455-38-9	3.02	4.24
435	c1c(F)c(C(=O)O)ccc1	445-29-4	2.26	3.28
436	c1c(O)c(C(F)(F)F)ccc1	444-30-4	3.83	3.70
437	FC(F)(F)c1ccc(O)cc1	402-45-9	3.86	3.59
438	ClC=CCCl	10061-01-5	2.82	2.35
439	c1c(I)cc(C(=O)O)cc1	618-51-9	4.28	1.66
440	c1c(I)c(C(=O)O)ccc1	88-67-5	3.28	3.46
441	NC(=S)c1cc(I)c(O)c(I)c1	3337-68-6	4.38	4.74
442	N1=Cc2ccccc2O1	271-95-4	2.23	3.93
443	N1=C2C=CC=CC2=CO1	271-58-9	2.08	3.53
444	C1=Nc2ccccc2O1	273-53-0	2.17	2.28
445	ClC=CCCl	10061-02-6	2.78	2.35
446	ClC(Cl)C(F)(F)OC	76-38-0	3.02	1.96
447	CC(Cl)(Cl)C(=O)O	75-99-0	1.83	1.70
448	N1C(=O)NC(=O)C1	461-72-3	-2.31	-2.18
449	BrCC=C	106-95-6	2.45	1.91
450	C=C(C)Cl	557-98-2	2.74	2.35
451	ICI	75-11-6	3.15	2.96
452	CCN=C=S	542-85-8	2.01	2.49
453	N1C=C(N)C=N1	28466-26-4	-1.49	-0.14
454	CC=C	115-07-1	2.42	2.44
455	BrCCCCl	109-70-6	2.98	2.34
456	BrCCCBr	109-64-8	3.24	3.39
457	ClCCCCl	142-28-9	2.74	2.36
458	ClCC(Cl)C	78-87-5	2.76	2.49
459	ICCCI	627-31-6	4.13	4.72
460	Nc1nc(N)nc(N)n1	108-78-1	-1.87	-2.01
461	CBr	74-83-9	1.63	0.96
462	CCCBr	106-94-5	2.87	2.46
463	CC(Br)C	75-26-3	2.87	2.43
464	CC(Cl)C	75-29-6	2.60	2.43
465	CCCCl	540-54-5	2.79	3.03
466	CC(I)C	75-30-9	3.95	3.30
467	CCCI	107-08-4	3.47	3.10
468	O=CN(C)C	68-12-2	-1.38	-1.01
469	CC(=O)NC	79-16-3	-1.44	-0.89
470	NC(C)C(=O)O	56-41-7	-3.90	-2.21

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
471	NC(C)C(=O)O	302-72-7	-4.05	-2.21
472	CNCC(=O)O	107-97-1	-3.80	-2.28
473	OCC(N)C(=O)O	56-45-1	-4.55	-4.40
474	CCC	74-98-6	3.23	2.90
475	CCC(=O)NN	5818-15-5	-1.37	-0.90
476	OCCCO	504-63-2	-1.42	-2.21
477	OCC(O)CO	56-81-5	-2.41	-2.26
478	CCCS	107-03-9	2.48	2.50
479	CCSC	624-89-5	2.10	1.58
480	CI	74-88-4	2.06	1.67
481	NCCCO	156-87-6	-1.53	-0.89
482	NNC(=O)N(C)C	40685-92-5	-2.15	-3.17
483	NCCCN	109-76-2	-1.95	-2.08
484	ClC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	87-68-3	6.54	4.29
485	ClC(F)(F)F	75-72-9	2.26	2.38
486	O=CN	75-12-7	-2.06	-2.14
487	S1C(Br)=C(Br)C=C1	3140-93-0	4.83	4.45
488	n1cc(Cl)nc(F)c1	33873-10-8	1.57	1.71
489	n1cc(Cl)nc(Cl)c1	4774-14-5	2.09	1.62
490	n1c(Cl)ccnc1Cl	3934-20-1	1.59	1.74
491	C1=CC(Br)=CO1	22037-28-1	2.98	2.50
492	C1=CC(Br)=CS1	872-31-1	3.58	3.72
493	C1=CC=C(Br)S1	1003-09-4	3.76	3.62
494	C1=CC=C(Cl)S1	96-43-5	3.47	4.08
495	ClC1=CSC=C1	17249-80-8	3.49	3.77
496	FC(F)(F)C(F)(F)C(F)(F)CO	375-01-9	2.65	0.86
497	O=C1C2=C(N=NN2)N=CN1	2683-90-1	-2.69	-2.70
498	ClC(Cl)(Cl)c1nc(N)nc(N)n1	16088-73-6	1.70	0.93
499	NC(=O)N	57-13-6	-2.89	-2.23
500	C1=CN=CC(=O)N1	6270-63-9	-2.04	-1.02
501	C1=CC(=O)N=CN1	4562-27-0	-1.89	-1.00
502	C1=CC=NC(=O)N1	557-01-7	-2.21	-0.07
503	N1C(=O)NC(=O)C=C1	66-22-8	-1.46	-2.63
504	O=CNN	624-84-0	-2.80	-2.32
505	C1(=O)NC(=O)NC(=O)C1	67-52-7	-2.01	-2.00
506	N1=C(CC(=O)O)C(=O)ON1	26537-53-1	-2.27	-1.60
507	ONC(=O)N	127-07-1	-2.46	-2.30
508	O1C=CC=C1	110-00-9	1.83	1.70
509	O=C1C=C(C)SS1	3620-08-4	1.72	2.07
510	ClC(Cl)(F)F	75-71-8	2.95	2.88
511	NC(=S)N	62-56-6	-1.44	-0.95
512	S1C=CC=C1	110-02-1	2.48	3.11
513	S=C1C=C(C)SS1	3354-40-3	2.56	3.68

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
514	CCOC(=O)C(Cl)(Cl)Cl	515-84-4	3.27	2.71
515	CC(=O)OCC(F)(F)F	406-95-1	1.61	1.42
516	c1nc(C)nnc1	24108-33-6	-1.79	-2.41
517	C1=CC(N)=NC(=O)N1	71-30-7	-2.37	0.06
518	N1=C(C)N=C(C=NO)S1	61444-96-0	1.76	0.43
519	C=CC=C	106-99-0	2.72	2.48
520	BrCC(Br)C(Br)CBr	1529-68-6	4.40	3.13
521	NC(=O)NN	57-56-7	-3.76	-2.31
522	N1=C(O)C=C(CN)O1	2763-96-4	-3.27	-0.18
523	NNC	60-34-4	-1.44	-2.18
524	CC1=NSN=C1C	5728-21-2	1.75	0.98
525	NC(=O)C1=C(N)NC=N1	360-97-4	-1.50	-2.72
526	ClC(F)(F)C(F)(F)Cl	76-14-2	3.86	2.94
527	FC(Cl)(Cl)C(F)(F)Cl	76-13-1	4.32	3.13
528	OC(=O)C(O)CC(=O)O	6915-15-7	-1.72	-2.24
529	OC(=O)C(O)C(O)C(=O)O	87-69-4	-1.64	-1.88
530	BrCCC=C	5162-44-7	3.20	3.30
531	CCC(Br)C(=O)O	80-58-0	1.94	1.36
532	CC(=O)OCCBr	927-68-4	1.52	1.42
533	[2H]C(Cl)(Cl)Cl	865-49-6	2.67	2.50
534	ClC(Cl)(Cl)C(O)(C)C	57-15-8	2.78	2.80
535	FC(F)(F)C(O)(C)C	507-52-8	1.42	1.31
536	OC(=O)C1CCN1	2517-04-6	-3.88	-2.37
537	OC(=O)C1(N)CC1	22059-21-8	-3.80	-2.27
538	OC(=O)C1CNC1	36476-78-5	-3.99	-2.21
539	ClC(Cl)=C(Cl)Cl	127-18-4	4.65	3.18
540	NC(C(=O)O)CC(=O)O	56-84-8	-5.03	-3.05
541	C1(=O)NC(=N)N(C)C1	60-27-5	-2.41	-1.59
542	ClC(Cl)(Cl)C(Cl)(Cl)Cl	67-72-1	5.66	4.83
543	C=C(C)C	115-11-7	3.21	2.52
544	CC=CC	624-64-6	3.16	3.26
545	CC=CC	590-18-1	3.19	3.26
546	C=CCC	106-98-9	3.28	2.93
547	ClCCCCCl	110-56-5	3.06	3.26
548	ClCCOCCCl	111-44-4	1.76	1.55
549	FC(F)(F)CN(C)C	819-06-7	1.45	1.40
550	CC(=O)NCC(=O)N	2620-63-5	-2.50	-1.70
551	NCC(=O)NCC(=O)O	556-50-3	-3.99	-4.00
552	NC(=O)CC(N)C(=O)O	70-47-3	-5.22	-2.80
553	FC(F)(F)C(F)(F)F	76-16-4	2.74	1.74
554	CCOC=C	109-92-2	1.42	1.65
555	CCCCBr	109-65-9	3.76	3.74
556	BrC(C)(C)C	507-19-7	1.57	3.45

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
557	CC(C)CBr	78-77-3	3.46	3.46
558	CCCCCl	109-69-3	3.61	3.15
559	CC(Cl)CC	78-86-4	3.45	3.35
560	FC(F)(F)C(Cl)Br	151-67-7	3.15	2.43
561	ClC(C)(C)C	507-20-0	3.27	3.26
562	CC(C)CCl	513-36-0	3.27	3.71
563	CCCCF	2366-52-1	3.53	2.47
564	CCCCI	542-69-8	4.21	4.37
565	N1N=C(Br)N=C1Br	7411-23-6	3.06	0.40
566	CC(C)(C)N=O	917-95-3	2.06	1.57
567	NCCCC(=O)O	56-12-2	-4.34	-2.27
568	CCC(N)C(=O)O	80-60-4	-3.46	-2.30
569	CN(C)CC(=O)O	1118-68-9	-3.98	-2.13
570	OC(C)C(N)C(=O)O	72-19-5	-4.07	-3.24
571	NNC(=O)NCC=C	57421-73-5	-2.12	-0.84
572	CCCC	106-97-8	3.95	3.38
573	CC(C)C	75-28-5	3.77	2.85
574	FC(Cl)(Cl)Cl	75-69-4	3.46	2.95
575	BrC=C(Br)Br	598-16-3	4.38	2.39
576	C1NCCNC1	110-85-0	-2.05	-1.02
577	FC(F)(F)C(Cl)F	2837-89-0	2.28	1.78
578	ClC=C(Cl)Cl	79-01-6	3.31	2.36
579	OCC(O)C(O)CO	7541-59-5	-3.13	-2.29
580	CCSCC	352-93-2	2.67	3.06
581	CCCCS	109-79-5	3.12	3.42
582	O=CC(Cl)(Cl)Cl	75-87-6	2.20	1.32
583	OCCNCCO	111-42-2	-1.95	-2.51
584	N=C(N)NC(=N)N(C)C	657-24-9	-1.95	-3.35
585	OC(=O)C(Cl)(Cl)Cl	76-03-9	1.82	1.72
586	C[Ge](C)(C)C	865-52-1	4.53	2.36
587	ClC(Cl)(Cl)C(Cl)Cl	76-01-7	4.40	3.94
588	C[Pb](C)(C)C	75-74-1	4.06	1.66
589	C[Si](C)(C)C	75-76-3	4.43	2.87
590	C[Sn](C)(C)C	594-27-4	4.76	1.64
591	n1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	2176-62-7	4.83	4.06
592	C1(Cl)=C(Cl)C(Cl)(Cl)C(Cl)=C1Cl	77-47-4	6.89	4.25
593	BrC1=NC2=C(Br)NC(Br)=NC2=N1	18874-52-7	4.21	1.75
594	c1(Cl)cc(Cl)cc(Cl)n1	16063-69-7	3.66	2.53
595	c1c(Cl)cc(Cl)c(Cl)n1	16063-70-0	4.25	2.67
596	FC(F)(F)C(F)F	354-33-6	1.83	1.77
597	c1(Cl)c(Cl)cc(Cl)c(O)n1	6515-38-4	4.39	2.81
598	c1c(Cl)ccc(Cl)n1	16110-09-1	3.28	2.68
599	c1c(Cl)cc(Cl)cn1	2457-47-8	3.50	1.95

TABLE S1: continued from previous page

#	SMILES	CAS	ΔG_{ow}^{exp}	ΔG_{ow}^{CG}
600	c1cc(Cl)nc(Cl)c1	2402-78-0	2.94	2.47
601	n1c(F)cccc1F	1513-65-1	1.60	1.72
602	c1cc(Br)cnc1	626-55-1	2.19	2.12
603	c1c(Br)ccnc1	1120-87-2	2.10	2.17
604	c1ccc(Br)nc1	109-04-6	1.91	1.98
605	c1c(Cl)ccnc1	626-61-9	1.75	2.02
606	c1cc(Cl)cnc1	626-60-8	1.82	1.85
607	c1ccc(Cl)nc1	109-09-1	1.67	2.58
608	FCC(F)(F)Cl	421-04-5	1.90	2.03
609	c1cc(I)cnc1	1120-90-7	2.46	2.65
610	N1C(=O)NC(=O)C(C=O)=C1	1195-08-0	-1.41	-3.49
611	ClC=CCl	156-59-2	2.54	1.79
612	C12=C(NC=N1)C(=O)NC=N2	68-94-0	-1.42	-0.63
613	N1C(C(=O)NC(=O)N2)=C2NC1=O	69-93-2	-3.99	-5.68
614	C1(C=O)=CSC=C1	498-62-4	1.38	2.07
615	C1=C(C=O)SC=C1	98-03-3	1.40	1.96
616	ClC=CCl	156-60-5	2.86	1.79
617	C1=C(C(=O)O)SC=C1	527-72-0	2.15	1.95
618	C1(C(=O)O)=CSC=C1	88-13-1	2.05	1.94
619	O=C1SSC(C(=O)C)=C1	620957-93-9	1.56	1.81
620	C=C(Cl)Cl	75-35-4	2.91	2.90
621	C1(C(=O)O)=COC=C1	488-93-7	1.41	1.04
622	n1c(C)cnc(Cl)c1	59303-10-5	1.48	1.75
623	n1cc(C)nc(Cl)c1	38557-71-0	1.41	0.17
624	n1cc(OC)nc(Cl)c1	33332-30-8	2.26	1.54
625	n1c(OC)cnc(Cl)c1	33332-31-9	2.08	1.90
626	CCOC1=NC(C(Cl)(Cl)Cl)=NS1	2593-15-9	3.49	2.31
627	ClC(Cl)(Cl)c1nc(C)nc(N)n1	21227-47-4	2.42	2.02
628	ClC(Cl)(Cl)c1nc(N)nc(OC)n1	115571-04-5	3.27	-1.38
629	ClC(Cl)(Cl)c1nc(N)nc(SC)n1	14946-02-2	4.27	1.37
630	FC(F)(F)C(F)(F)C(=O)OCC	426-65-3	2.90	2.65
631	ClC(Cl)C(Cl)Cl	79-34-5	3.27	3.23
632	NC(=S)C1=CC=CS1	20300-02-1	1.83	2.99
633	n1c(C(=O)N)nccc1	88511-48-2	-1.64	-1.86
634	ClC(Cl)(Cl)Cl	56-23-5	3.87	3.38
635	ClC(Cl)(Cl)CCl	630-20-6	3.64	3.29
636	C=C(F)F	75-38-7	1.70	2.50
637	O=C1NC(C)=CC=N1	15231-48-8	-1.98	-0.98
638	N1(C)C(=O)NC(=O)C=C1	615-77-0	-1.64	-2.29
639	n1cc(SC)ncc1	21948-70-9	1.60	1.25
640	n1c(SC)nccc1	823-09-6	1.38	1.01
641	C1=C(C)OC=C1	534-22-5	2.53	2.45
642	COC1=CC=CS1	16839-97-7	2.91	0.44

TABLE S1: continued from previous page

#	SMILES	CAS	$\Delta G_{\mathrm{ow}}^{\mathrm{exp}}$	$\Delta G_{\mathrm{ow}}^{\mathrm{CG}}$
643	CCC1=CC(=O)SS1	164584-61-6	2.31	2.67
644	CCC1=CSSC1=O	35659-69-9	2.60	2.62
645	CC1=C(C)SSC1=O	35659-69-9	2.37	2.07
646	C1=C(OC)OC=C1	25414-22-6	1.97	1.39
647	C1=C(C)SC=C1	554-14-3	3.19	3.83
648	C1(C)=CSC=C1	616-44-4	3.20	3.82
649	CCC1=CC(=S)SS1	52514-89-3	3.16	3.00
650	CCC1=CSSC1=S	7113-30-6	3.65	4.51
651	S=C1SSC(C)=C1C	3354-39-0	3.35	3.53
652	C=CBr	593-60-2	2.15	1.57
653	C1=CN(C)C=C1	96-54-8	1.65	1.73

TABLE S2: SMILES string, molecule name, and experimental and CG hydration free energy for all 354 neutral compounds used in this work. Units are in kcal/mol.

#	SMILES	Name	$\Delta G_{\mathrm{hydr}}^{\mathrm{exp}}$	$\Delta G_{\mathrm{hydr}}^{\mathrm{CG}}$
1	C(C(Cl)(Cl)Cl)Cl	1112-tetrachloroethane	-1.28	-2.86
2	CC(Cl)(Cl)Cl	111-trichloroethane	-0.19	1.87
3	C[C@@H](C(F)(F)F)O	111-trifluoropropan-2-ol	-4.16	-0.25
4	C(C(Cl)Cl)(Cl)Cl	1122-tetrachloroethane	-2.47	-1.23
5	C(C(F)(Cl)Cl)(F)(F)Cl	112-trichloro-122-trifluoroethane	1.77	-3.48
6	C(C(Cl)Cl)Cl	112-trichloroethane	-1.99	-3.89
7	C(=O)(C)OC(C)OC(=O)C	11-diacetoxyethane	-4.97	-12.00
8	CC(Cl)Cl	11-dichloroethane	-0.84	0.48
9	C=C(Cl)Cl	11-dichloroethene	0.25	0.50
10	CCOC(C)OCC	11-diethoxyethane	-3.28	-6.49
11	CC(F)F	11-difluoroethane	-0.11	-1.19
12	c1c(cc(c(c1Cl)Cl)Cl)Cl	1235-tetrachlorobenzene	-1.62	-8.28
13	c1cc(c(c(c1)C)C)C	123-trimethylbenzene	-1.21	-5.26
14	c1c(c(cc(c1Cl)Cl)Cl)Cl	1245-tetrachlorobenzene	-1.34	-8.35
15	c1cc(c(cc1Cl)Cl)Cl	124-trichlorobenzene	-1.12	-9.26
16	c1cc(c(cc1C)C)C	124-trimethylbenzene	-0.86	-4.63
17	C(=O)(C)OCCOC(=O)C	12-diacetoxyethane	-6.34	-11.10
18	C(CBr)Br	12-dibromoethane	-2.33	-3.33
19	c1ccc(c(c1)Cl)Cl	12-dichlorobenzene	-1.36	-5.25
20	C(CCl)Cl	12-dichloroethane	-1.79	-4.64
21	C[C@@H](CCl)Cl	12-dichloropropane	-1.27	-3.83
22	CCOCCOCC	12-diethoxyethane	-3.54	-7.37
23	COCCOC	12-dimethoxyethane	-4.84	-3.36
24	C(CO)O	12-ethanediol	-9.30	-4.41

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
25	c1c(cc(cc1Cl)Cl)Cl	135-trichlorobenzene	-0.78	-4.66
26	c1c(cc(cc1C)C)C	135-trimethylbenzene	-0.90	-4.62
27	c1cc(cc(c1)Cl)Cl	13-dichlorobenzene	-0.98	-5.41
28	C(CCl)CCl	13-dichloropropane	-1.89	-2.88
29	c1cc(ccc1Cl)Cl	14-dichlorobenzene	-1.01	-10.00
30	C(CCCl)CCl	14-dichlorobutane	-2.32	-2.32
31	C1CN(CCN1C)C	14-dimethyl-piperazine	-7.58	-3.29
32	C1COCCO1	14-dioxane	-5.06	-7.77
33	C(CBr)Cl	1-bromo-2-chloroethane	-1.95	-4.29
34	CC(C)CBr	1-bromo-2-methylpropane	-0.03	-2.92
35	CCCCBr	1-bromobutane	-0.40	-2.70
36	CCCCCCCBr	1-bromoheptane	0.34	-3.01
37	CCCCCCBr	1-bromohexane	0.18	-4.64
38	CCCCCCCCBr	1-bromooctane	0.52	-4.08
39	CCCCCBr	1-bromopentane	-0.10	-1.49
40	CCCBr	1-bromopropane	-0.56	-3.53
41	C(C(F)(F)F)Cl	1-chloro-222-trifluoroethane	0.06	-4.76
42	CCCCCl	1-chlorobutane	-0.16	-3.19
43	CCCCCCCCl	1-chloroheptane	0.29	-0.21
44	CCCCCCCl	1-chlorohexane	0.00	0.05
45	CCCCCCl	1-chloropentane	-0.07	-2.53
46	CCCCI	1-iodobutane	-0.25	-1.63
47	CCCCCCCI	1-iodoheptane	0.27	-1.82
48	CCCCCCI	1-iodohexane	0.08	-3.66
49	CCCCCI	1-iodopentane	-0.14	-0.49
50	CCCI	1-iodopropane	-0.53	-2.49
51	C1=C(CCCC1)C	1-methylcyclohexene	0.67	-1.26
52	c1cn(cn1)C	1-methyl-imidazole	-8.41	-9.70
53	c1ccn(c1)C	1-methyl-pyrrole	-2.89	-5.30
54	C(C(F)(F)F)O	222-trifluoroethanol	-4.31	-2.20
55	CC(C)CC(C)(C)C	224-trimethylpentane	2.89	-1.45
56	CC(C)CCC(C)(C)C	225-trimethylhexane	2.93	-0.16
57	CCC(C)(C)C	22-dimethylbutane	2.51	1.85
58	CCCC(C)(C)C	22-dimethylpentane	2.88	-1.52
59	CC(C)(C)C	22-dimethylpropane	2.51	1.84
60	CC(C)C(C)C(C)C	234-trimethylpentane	2.56	0.07
61	C=C(C(=C)C)C	23-dimethylbuta-13-diene	0.40	1.91
62	CC(C)C(C)C	23-dimethylbutane	2.34	1.81
63	CC[C@@H](C)C(C)C	23-dimethylpentane	2.52	-0.16
64	c1cc(c(c(c1)O)C)C	23-dimethylphenol	-6.16	-6.14
65	c1cc(c(C)nc1)C	23-dimethylpyridine	-4.82	-10.34
66	C(=O)(C(C)C)C(C)C	24-dimethylpentan-3-one	-2.74	-4.18
67	CC(C)CC(C)C	24-dimethylpentane	2.83	-1.40

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
68	c1cc(c(cc1C)C)O	24-dimethylphenol	-6.01	-6.13
69	c1cnc(cc1C)C	24-dimethylpyridine	-4.86	-10.34
70	c1cc(c(cc1C)O)C	25-dimethylphenol	-5.91	-6.22
71	c1cc(C)ncc1C	25-dimethylpyridine	-4.72	-9.26
72	C1C[C@H](C)O[C@H]1C	25-dimethyltetrahydrofuran	-2.92	-5.68
73	c1cc(c(c(c1)C)N)C	26-dimethylaniline	-5.21	-6.22
74	c1cc(cc2ccc(cc12)C)C	26-dimethylnaphthalene	-2.63	-7.40
75	c1cc(c(c(c1)C)O)C	26-dimethylphenol	-5.26	-6.13
76	c1cc(C)nc(c1)C	26-dimethylpyridine	-4.59	-9.50
77	CC(C)(C)Br	2-bromo-2-methylpropane	0.84	1.87
78	CC(C)Br	2-bromopropane	-0.48	0.52
79	CCCCOCCO	2-butoxyethanol	-6.25	-3.71
80	COC(CCl)(OC)OC	2-chloro-111-trimethoxyethane	-4.59	-7.23
81	CC(C)(C)Cl	2-chloro-2-methylpropane	1.09	1.34
82	c1ccc(c(c1)N)Cl	2-chloroaniline	-4.91	-6.91
83	CC[C@H](C)Cl	2-chlorobutane	0.00	1.23
84	c1ccc(c(c1)O)Cl	2-chlorophenol	-4.55	-6.99
85	CC(C)Cl	2-chloropropane	-0.25	0.49
86	c1ccnc(c1)Cl	2-chloropyridine	-4.39	-9.63
87	c1ccc(c(c1)C)Cl	2-chlorotoluene	-1.14	-5.30
88	CCOCCO	2-ethoxyethanol	-6.69	-3.29
89	c1cnc(cn1)CC	2-ethylpyrazine	-5.45	-13.50
90	c1ccnc(c1)CC	2-ethylpyridine	-4.33	-9.54
91	c1ccc(c(c1)C)CC	2-ethyltoluene	-1.04	-5.25
92	c1ccc(c(c1)O)F	2-fluorophenol	-5.29	-7.88
93	c1ccc(c(c1)O)I	2-iodophenol	-6.20	-6.60
94	CC(C)I	2-iodopropane	-0.46	1.90
95	c1ccc(c(c1)N)OC	2-methoxyaniline	-6.12	-14.21
96	COCCN	2-methoxyethanamine	-6.55	-3.24
97	c1ccc(c(c1)O)OC	2-methoxyphenol	-5.57	-14.25
98	C(=C(C)C)C	2-methyl-but-2-ene	1.31	1.92
99	C(=C(C)C)C	2-methylbut-2-ene	1.31	1.92
100	C=CC(=C)C	2-methylbuta-13-diene	0.68	0.57
101	CC[C@@H](C)CO	2-methylbutan-1-ol	-4.42	-0.35
102	CCC(C)(C)O	2-methylbutan-2-ol	-4.43	-0.24
103	CCC(C)C	2-methylbutane	2.38	1.93
104	CCCCC(C)C	2-methylhexane	2.93	-0.22
105	C=C(C)CCC	2-methylpent-1-ene	1.47	1.91
106	CCCC(C)(C)O	2-methylpentan-2-ol	-3.92	-5.36
107	CC[C@H](C(C)C)O	2-methylpentan-3-ol	-3.88	0.52
108	CCCC(C)C	2-methylpentane	2.51	1.91
109	CC(C)CO	2-methylpropan-1-ol	-4.50	-2.26
110	CC(C)(C)O	2-methylpropan-2-ol	-4.47	-2.22

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
111	C=C(C)C	2-methylpropene	1.16	0.56
112	c1cnc(cn1)C	2-methylpyrazine	-5.51	-15.78
113	c1ccnc(c1)C	2-methylpyridine	-4.63	-10.35
114	C1C[C@H](C)OC1	2-methyltetrahydrofuran	-3.30	-1.15
115	c1cc(C)sc1	2-methylthiophene	-1.38	-2.29
116	c1ccc(cc1)CCO	2-phenylethanol	-6.79	-6.76
117	CCCOCCO	2-propoxyethanol	-6.40	-2.14
118	C(#N)CC(OC)(OC)OC	333-trimethoxypropionitrile	-6.40	-6.31
119	C(=O)(C)C(C)(C)C	33-dimethylbutan-2-one	-3.11	-5.70
120	CCC(C)(C)CC	33-dimethylpentane	2.56	1.89
121	c1cc(cc(c1C)C)O	34-dimethylphenol	-6.50	-6.16
122	c1cncc(c1C)C	34-dimethylpyridine	-5.22	-10.46
123	c1c(cc(cc1C)O)C	35-dimethylphenol	-6.27	-6.09
124	c1c(cncc1C)C	35-dimethylpyridine	-4.84	-10.29
125	c1cc(cc(c1)Cl)N	3-chloroaniline	-5.82	-6.80
126	c1cc(cc(c1)Cl)O	3-chlorophenol	-6.62	-7.05
127	C=CCCl	3-chloroprop-1-ene	-0.57	0.55
128	c1cc(cnc1)Cl	3-chloropyridine	-4.01	-10.44
129	c1cc(cc(c1)O)CC	3-ethylphenol	-6.25	-6.92
130	c1cc(cnc1)CC	3-ethylpyridine	-4.59	-9.56
131	c1cc(cnc1)C=O	3-formylpyridine	-7.10	-12.43
132	c1cc(cc(c1)O)C=O	3-hydroxybenzaldehyde	-9.50	-7.56
133	c1cc(cc(c1)OC)N	3-methoxyaniline	-7.29	-7.71
134	c1cc(cc(c1)OC)O	3-methoxyphenol	-7.66	-7.64
135	c1ccc2c(c1)c(c[nH]2)C	3-methyl-1h-indole	-5.88	-13.11
136	C=CC(C)C	3-methyl-but-1-ene	1.83	1.31
137	C=CC(C)C	3-methylbut-1-ene	1.82	1.31
138	CC(C)CCO	3-methylbutan-1-ol	-4.42	-5.36
139	C(=O)(C)C(C)C	3-methylbutan-2-one	-3.24	-2.11
140	C(=O)(CC(C)C)O	3-methylbutanoic-acid	-6.09	-5.45
141	CCCC[C@@H](C)CC	3-methylheptane	2.97	1.10
142	CCC[C@H](C)CC	3-methylhexane	2.71	1.90
143	CCC(C)CC	3-methylpentane	2.51	1.84
144	c1cc(cnc1)C	3-methylpyridine	-4.77	-10.27
145	c1cc(ccc1O)Br	4-bromophenol	-7.13	-11.20
146	c1cc(ccc1C)Br	4-bromotoluene	-1.39	-9.49
147	c1cc(c(cc1O)C)Cl	4-chloro-3-methylphenol	-6.79	-10.63
148	c1cc(ccc1N)Cl	4-chloroaniline	-5.90	-6.85
149	c1cc(ccc1O)Cl	4-chlorophenol	-7.03	-6.97
150	c1cc(ccc1CC)O	4-ethylphenol	-6.13	-6.90
151	c1cnccc1CC	4-ethylpyridine	-4.73	-9.62
152	c1cc(ccc1C)CC	4-ethyltoluene	-0.95	-5.26
153	c1cc(ccc1O)F	4-fluorophenol	-6.19	-7.73

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
154	c1cnccc1C=O	4-formylpyridine	-7.00	-12.46
155	c1cc(ccc1C=O)O	4-hydroxybenzaldehyde	-8.83	-7.76
156	c1cc(ccc1N)OC	4-methoxyaniline	-7.48	-7.66
157	c1c(C)nc[nH]1	4-methyl-1h-imidazole	-10.27	-9.88
158	c1cc(ccc1C=O)C	4-methylbenzaldehyde	-4.27	-6.20
159	CC(C)C[C@@H](C)O	4-methylpentan-2-ol	-3.73	-5.36
160	C(=O)(C)CC(C)C	4-methylpentan-2-one	-3.05	-5.54
161	c1cnccc1C	4-methylpyridine	-4.93	-10.25
162	c1cc(ccc1CCC)O	4-n-propylphenol	-5.90	-5.61
163	C(=O)C	acetaldehyde	-3.50	-3.35
164	C(=O)(C)O	acetic-acid	-6.69	-3.39
165	C(#N)C	acetonitrile	-3.88	-0.22
166	c1ccc(cc1)C(=C)C	alpha-methylstyrene	-1.24	-6.05
167	c1ccc(cc1)OC	anisole	-2.45	-6.93
168	C1CNC1	azetidine	-5.56	-3.39
169	c1ccc(cc1)CO	benzyl-alcohol	-6.62	-7.63
170	c1ccc(cc1)CBr	benzyl-bromide	-2.38	-9.39
171	C(F)(F)(F)Br	bromotrifluoromethane	1.79	0.59
172	C#CCC	but-1-yne	-0.16	0.54
173	C(#N)CCC	butanenitrile	-3.64	1.92
174	C(=O)CCC	butanone	-3.71	-0.20
175	C(F)(F)Cl	chlorodifluoromethane	-0.50	-0.27
176	C=CCl	chloroethylene	-0.59	-0.26
177	C(F)Cl	chlorofluoromethane	-0.77	-1.08
178	C1CC[C@@H]([C@@H](C1)C)C	cis-12-dimethylcyclohexane	1.58	-0.67
179	C1=CC=CCC=C1	cyclohepta-135-triene	-0.99	-0.95
180	C1CCCC(CC1)O	cycloheptanol	-5.48	-8.53
181	C1CCC(CC1)O	cyclohexanol	-5.46	-5.05
182	C1(=O)CCCCC1	cyclohexanone	-4.91	-0.19
183	C1CCC(CC1)N	cyclohexylamine	-4.59	-4.66
184	C1CCC(C1)O	cyclopentanol	-5.49	-6.50
185	C1(=O)CCCC1	cyclopentanone	-4.70	-2.06
186	C1=CCCC1	cyclopentene	0.56	0.50
187	CCCCCCCCCCO	decan-1-ol	-3.64	-4.05
188	C(Br)Br	dibromomethane	-1.96	-0.35
189	C(Cl)Cl	dichloromethane	-1.31	-0.30
190	CCNCC	diethylamine	-4.07	-2.16
191	CCSSCC	diethyl-disulfide	-1.64	-2.66
192	CCOCC	diethyl-ether	-1.59	-0.21
193	C(=O)(CC(=O)OCC)OCC	diethyl-malonate	-6.00	-10.98
194	C(=O)(CCC(=O)OCC)OCC	diethyl-succinate	-5.71	-13.79
195	CCSCC	diethyl-sulfide	-1.46	-3.12
196	C(I)I	diiodomethane	-2.49	0.58

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
197	CC(C)NC(C)C	diisopropylamine	-3.22	-0.22
198	CC(C)OC(C)C	diisopropyl-ether	-0.53	-5.89
199	CC(C)SC(C)C	di-isopropyl-sulfide	-1.21	-1.08
200	COCOC	dimethoxymethane	-2.93	-3.23
201	CNC	dimethylamine	-4.29	-3.26
202	COC	dimethyl-ether	-1.91	-3.32
203	CSC	dimethyl-sulfide	-1.61	-1.15
204	CS(=O)(=O)C	dimethyl-sulfone	-10.08	-3.23
205	CS(=O)C	dimethyl-sulfoxide	-8.71	-3.22
206	CCCCNCCCC	di-n-butylamine	-3.24	-1.85
207	CCCCOCCCC	di-n-butyl-ether	-0.83	-6.55
208	CCCNCCC	di-n-propylamine	-3.65	0.54
209	CCCOCCC	di-n-propyl-ether	-1.16	0.62
210	CCCSCCC	di-n-propyl-sulfide	-1.28	-1.40
211	C(=C\Cl)/Cl	E-12-dichloroethene	-0.78	-4.66
212	C(=C\C)/C=O	E-but-2-enal	-4.22	-1.12
213	C(=C\CCCC)/C	E-hept-2-ene	1.68	1.84
214	C(=C\CCC)/C=O	E-hex-2-enal	-3.68	0.55
215	C(=C\CCCCC)/C=O	E-oct-2-enal	-3.43	-1.25
216	C(=O)(C)N	ethanamide	-9.71	-3.38
217	c1ccc(cc1)OCC	ethyl-phenyl-ether	-2.22	-6.09
218	c1ccc(cc1)F	fluorobenzene	-0.80	-6.99
219	C=O	formaldehyde	-2.75	-3.23
220	[C@@H](C(F)(F)F)(Cl)Br	halothane	-0.11	-4.30
221	C=CCCCCC	hept-1-ene	1.66	-0.76
222	C#CCCCCC	hept-1-yne	0.60	1.90
223	CCCCCCCO	heptan-1-ol	-4.21	-3.20
224	C(=O)(C)CCCCC	heptan-2-one	-3.04	-4.13
225	C(=O)(CCC)CCC	heptan-4-one	-2.92	-4.24
226	C(=O)CCCCCC	heptanal	-2.67	-2.90
227	C=CCCCC	hex-1-ene	1.58	1.86
228	C(#C)CCCC	hex-1-yne	0.29	1.82
229	C=CCCC=C	hexa-15-diene	1.01	1.87
230	C(=C(F)F)(C(F)(F)F)F	hexafluoropropene	-3.76	-11.75
231	CCCCCCO	hexan-1-ol	-4.40	-3.41
232	C(=O)(C)CCCC	hexan-2-one	-3.28	-4.57
233	CCC[C@H](CC)O	hexan-3-ol	-4.06	-4.39
234	C(=O)CCCCC	hexanal	-2.81	-4.21
235	C(=O)(CCCCC)O	hexanoic-acid	-6.21	-3.23
236	c1ccc2c(c1)CCC2	indane	-1.46	-8.60
237	c1ccc(cc1)I	iodobenzene	-1.74	-5.90
238	CCI	iodoethane	-0.74	1.25
239	C(=O)(C)OCCC(C)C	isoamyl-acetate	-2.21	-8.03

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
240	C(=O)OCCC(C)C	isoamyl-formate	-2.13	-4.31
241	C(=O)(C)OCC(C)C	isobutyl-acetate	-2.36	-4.21
242	C(=O)OCC(C)C	isobutyl-formate	-2.22	-5.54
243	C(=O)(C(C)C)OCC(C)C	isobutyl-isobutanoate	-1.69	-13.81
244	C(=O)C(C)C	isobutyraldehyde	-2.86	-2.20
245	[C@@H](C(F)(F)F)(OC(F)F)Cl	isoflurane	0.10	-4.29
246	C(=O)(C)OC(C)C	isopropyl-acetate	-2.64	-5.57
247	c1ccc(cc1)C(C)C	isopropylbenzene	-0.30	-4.90
248	C(=O)OC(C)C	isopropyl-formate	-2.02	-1.25
249	c1cc(cc(c1)O)C	m-cresol	-5.49	-7.12
250	CS(=O)(=O)Cl	methanesulfonyl-chloride	-4.87	-3.21
251	CS	methanethiol	-1.24	-2.20
252	COC(C(Cl)Cl)(F)F	methoxyflurane	-1.12	-5.34
253	C(=O)(C)OC	methyl-acetate	-3.13	-2.13
254	C(=O)(CCC)OC	methyl-butanoate	-2.83	-5.55
255	C(=O)(CCl)OC	methyl-chloroacetate	-4.00	-7.11
256	C(#N)CC(=O)OC	methyl-cyanoacetate	-6.72	-6.52
257	C(=O)(C1CCCCC1)OC	methyl-cyclohexanecarboxylate	-3.30	-8.08
258	C(=O)(C1CCCCC1)C	methyl-cyclohexyl-ketone	-3.90	-8.08
259	C1CCC(C1)C	methylcyclopentane	1.59	-1.72
260	C(=O)(C1CC1)OC	methyl-cyclopropanecarboxylate	-4.10	-6.28
261	C(=O)(C1CC1)C	methyl-cyclopropyl-ketone	-4.61	-1.12
262	CCOC	methyl-ethyl-ether	-2.10	-2.14
263	CCSC	methyl-ethyl-sulfide	-1.50	-0.33
264	C(=O)OC	methyl-formate	-2.78	-3.39
265	C(=O)(CCCCC)OC	methyl-hexanoate	-2.49	-8.02
266	CC(C)OC	methyl-isopropyl-ether	-2.01	-2.20
267	COS(=O)(=O)C	methyl-methanesulfonate	-4.87	-3.27
268	C(=O)(CCCCCCC)OC	methyl-octanoate	-2.04	-5.40
269	C(=O)(CCCC)OC	methyl-pentanoate	-2.56	-4.37
270	C(=O)(CC)OC	methyl-propanoate	-2.93	-2.27
271	CCCOC	methyl-propyl-ether	-1.66	-1.16
272	CC(C)(C)OC	methyl-t-butyl-ether	-2.21	0.53
273	CC(C)(C)OC	methyl-tert-butyl-ether	-2.21	0.53
274	C(=O)(C(C)(C)C)OC	methyl-trimethylacetate	-2.40	-5.60
275	c1cc(cc(c1)C)C	m-xylene	-0.83	-5.43
276	C(=O)(C)N1CCCC1	N-acetylpyrrolidine	-9.80	-3.35
277	CCCCS	n-butanethiol	-0.99	1.88
278	C(=O)(CCCCC)N	n-butylacetamide	-9.31	-3.72
279	C(=O)(C)OCCCC	n-butyl-acetate	-2.64	-2.85
280	CCCCCCCCCC	n-decane	3.16	1.88
281	CCCCCCC	n-heptane	2.67	0.35
282	CCCCCCCN	n-heptylamine	-3.79	-2.17

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
283	CCCCCC	n-hexane	2.48	1.92
284	C(=O)(C)OCCCCCC	n-hexyl-acetate	-2.26	-6.76
285	CCCCCCN	n-hexylamine	-3.95	-3.40
286	C(=O)(C)NC	N-methylacetamide	-10.00	-3.19
287	c1ccc(cc1)NC	N-methylaniline	-4.69	-7.09
288	C1COCCN1C	N-methylmorpholine	-6.32	-3.33
289	C1CN(CCN1)C	N-methylpiperazine	-7.77	-8.46
290	C1CCN(CC1)C	N-methylpiperidine	-3.88	-4.82
291	c1ccc(cc1)C(=O)N(C)C	NN-dimethylbenzamide	-9.29	-0.14
292	C(=O)N(C)C	NN-dimethylformamide	-7.81	-3.23
293	c1cc(ccc1C(=O)N(C)C)C	NN-dimethyl-p-methylbenzamide	-9.76	-10.98
294	CCCCCCCCC	n-nonane	3.13	1.87
295	CCCCCCCC	n-octane	2.88	-0.29
296	CCCCCCCCN	n-octylamine	-3.65	-1.78
297	C=CCCCCCCC	non-1-ene	2.06	0.52
298	CCCCCCCCCO	nonan-1-ol	-3.88	-2.28
299	C(=O)(C)CCCCCCC	nonan-2-one	-2.49	-6.03
300	C(=O)(CCCC)CCCC	nonan-5-one	-2.64	-6.55
301	C(=O)CCCCCCCC	nonanal	-2.07	-3.86
302	CCCCC	n-pentane	2.32	1.85
303	C(=O)(C)OCCCCC	n-pentyl-acetate	-2.51	-8.12
304	CCCCCN	n-pentylamine	-4.09	-0.28
305	C1CCC(C1)CCCCC	n-pentylcyclopentane	2.55	-2.24
306	C(=O)(CC)OCCCCC	n-pentyl-propanoate	-2.11	-7.10
307	CCCS	n-propanethiol	-1.06	0.56
308	C(=O)(C)OCCC	n-propyl-acetate	-2.79	-5.50
309	c1ccc(cc1)CCC	n-propylbenzene	-0.53	-4.74
310	C(=O)(CCC)OCCC	n-propyl-butyrate	-2.28	-4.45
311	C1CCC(C1)CCC	n-propylcyclopentane	2.13	-0.15
312	C(=O)OCCC	n-propyl-formate	-2.48	-6.53
313	C(=O)(CC)OCCC	n-propyl-propanoate	-2.44	-4.34
314	c1ccc(c(c1)C)O	o-cresol	-5.87	-7.07
315	C=CCCCCC	oct-1-ene	1.92	-0.17
316	C#CCCCCC	oct-1-yne	0.71	1.85
317	CCCCCCCO	octan-1-ol	-4.09	-1.81
318	C(=O)(C)CCCCCC	octan-2-one	-2.88	-7.99
319	C(=O)CCCCCCC	octanal	-2.29	-0.30
320	c1ccc(c(c1)C)N	o-toluidine	-5.53	-6.93
321	c1ccc(c(c1)C)C	o-xylene	-0.90	-5.32
322	c1cc(ccc1C)O	p-cresol	-6.13	-6.99
323	c1cc(ccc1Br)Br	p-dibromobenzene	-2.30	-9.53
324	C#CCCC	pent-1-yne	0.01	1.84
325	C=CCC=C	penta-14-diene	0.93	1.36

TABLE S2: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$
326	C(C(Cl)(Cl)Cl)(Cl)Cl	pentachloroethane	-1.39	-1.50
327	CCCCCO	pentan-1-ol	-4.57	-0.37
328	C(=O)CCCC	pentanal	-3.03	-0.32
329	C(#N)CCCC	pentanenitrile	-3.52	1.90
330	C(=O)(CCCC)O	pentanoic-acid	-6.16	-4.58
331	c1ccc(cc1)SC	phenyl-methyl-sulfide	-2.73	-6.09
332	C=CCO	prop-2-en-1-ol	-5.03	-3.22
333	C(#N)CC	propanenitrile	-3.84	0.51
334	C(=O)(CC)O	propanoic-acid	-6.46	-2.20
335	C(=O)(C)C	propanone	-3.80	-3.27
336	C(=O)CC	propionaldehyde	-3.43	-2.14
337	C#CC	propyne	-0.48	-0.22
338	c1cc(ccc1C)N	p-toluidine	-5.57	-2.78
339	c1cc(ccc1C)C	p-xylene	-0.80	-5.47
340	[C@@H](C(F)(F)F)(F)Br	teflurane	0.50	-5.23
341	C(=C(Cl)Cl)(Cl)Cl	tetrachloroethene	0.10	-1.10
342	C(Cl)(Cl)(Cl)Cl	tetrachloromethane	0.08	1.84
343	C(F)(F)(F)F	tetrafluoromethane	3.12	0.55
344	C1CCOCC1	tetrahydropyran	-3.12	-5.21
345	c1ccc(cc1)S	thiophenol	-2.55	-6.32
346	C(Br)(Br)Br	tribromomethane	-2.13	1.86
347	C(=C(Cl)Cl)Cl	trichloroethene	-0.44	-3.82
348	C(Cl)(Cl)Cl	trichloromethane	-1.08	0.53
349	CCN(CC)CC	triethylamine	-3.22	0.50
350	COC(OC)OC	trimethoxy-methane	-4.42	-3.26
351	CN(C)C	trimethylamine	-3.20	-3.34
352	C(=O)(C)CCCCCCCCC	undecan-2-one	-2.15	-8.48
353	C(=C\Cl)\Cl	Z-12-dichloroethene	-1.17	-4.71
354	C(=C\CC)\C	Z-pent-2-ene	1.31	1.87

TABLE S3: SMILES string, molecule name, experimental and CG hydration free energy, and experimental and CG solvation in octanol free energy for all 69 neutral compounds used in this work. Units are in kcal/mol.

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{exp}}_{\mathrm{solv}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{solv}}$
1	CC=O	acetaldehyde	-3.55	-3.21	-3.64	-2.76
2	CCCCCC	hexane	2.49	1.92	-2.85	-1.50
3	CCC=O	propanal	-3.49	-2.14	-4.29	-2.71
4	C1CCCCC1	cyclohexane	1.23	-2.11	-2.68	-10.87
5	O=CC1=CC=CC=C1	benzaldehyde	-4.09	-6.95	-6.11	-11.12

TABLE S3: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{exp}}_{\mathrm{solv}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{solv}}$
6	CC=C	propene	1.29	0.55	-1.14	-1.89
7	CC(C)=O	acetone	-3.86	-3.35	-3.53	-2.68
8	C=CC=C	1,3-butadiene	0.57	0.52	-2.15	-1.96
9	CCC(C)=O	butanone	-3.72	-2.25	-4.12	-2.73
10	CCCC#C	1-pentyne	0.01	1.85	-2.69	-1.52
11	C1CCOC1	tetrahydrofuran	-3.51	-2.24	-4.14	-2.76
12	C1CCC=CC1	cyclohexene	0.37	-1.02	-3.54	-6.32
13	CC(O)=O	acetic acid	-6.80	-3.34	-6.56	-2.77
14	CCCl	ethyl chloride	-0.64	-0.19	-2.60	-1.97
15	COC(C)=O	methyl acetate	-3.32	-2.23	-3.57	-2.77
16	CC(Cl)(Cl)Cl	1,1,1-trichloroethane	-0.19	1.87	-3.60	-1.54
17	CCCCl	1-chloropropane	-0.27	0.60	-3.06	-2.43
18	ClCCCl	1,2-dichloroethane	-1.75	-4.63	-3.77	-6.48
19	CC	ethane	1.83	-0.28	-0.64	-1.93
20	CCOC(C)=O	ethyl acetate	-2.95	-6.38	-3.95	-7.21
21	Cl\C=C/Cl	cis-1,2-dichloroethene	-0.70	-4.70	-3.24	-6.45
22	CN	methylamine	-4.58	-3.37	-3.80	-2.26
23	Cl\C=C\Cl	trans-1,2-dichloroethene	-0.78	-4.76	-3.50	-6.55
24	CCN	ethylamine	-4.51	-3.36	-4.34	-2.77
25	ClC=C(Cl)Cl	trichloroethene	-0.44	-3.96	-3.75	-6.32
26	CNC	dimethylamine	-4.31	-3.26	-3.79	-2.79
27	C1=CC=CC=C1	benzene	-0.90	-6.91	-3.81	-11.08
28	C1CCNCC1	piperidine	-5.11	-1.09	-6.26	-2.10
29	CC1=CC=CC=C1	toluene	-0.77	-6.25	-4.50	-11.04
30	COCOC	dimethoxymethane	-2.98	-3.23	-3.23	-2.66
31	CN(C)C	trimethylamine	-3.24	-3.34	-3.46	-2.69
32	CN1CCCC1	1-methylpyrollidine	-4.03	-2.16	-5.29	-2.75
33	C1COCCN1	morpholine	-7.19	-9.04	-6.02	-7.83
34	NC1=CC=CC=C1	aniline	-4.91	-7.73	-6.14	-11.25
35	CCC	propane	1.97	0.53	-1.26	-2.37
36	CC#N	acetonitrile	-3.95	-0.27	-3.49	-1.92
37	CCC#N	propionitrile	-3.91	0.49	-4.13	-2.37
38	FC1=CC=CC=C1	fluorobenzene	-0.78	-6.96	-3.88	-11.14
39	Clc1ccccc1	chlorobenzene	-1.03	-6.08	-4.98	-11.19
40	CC(N)=O	acetamide	-9.74	-3.21	-8.01	-2.30
41	BrC1=CC=CC=C1	bromobenzene	-1.46	-8.01	-5.55	-11.56
42	CNC(C)=O	N-methylacetamide	-10.10	-3.35	-8.67	-2.32
43	CO	methanol	-5.13	-4.40	-4.07	-2.31
44	COCCOC	1,2-dimethoxyethane	-4.85	-3.36	-4.57	-2.74
45	CN(C)C(C)=O	N,N-dimethylacetamide	-8.57	-3.26	-7.52	-2.36
46	CCO	ethanol	-5.02	-3.22	-4.60	-2.75
47	CCCO	1-propanol	-4.87	-2.19	-5.21	-2.80
48	CC(C)O	2-propanol	-4.76	-3.33	-4.83	-2.72

TABLE S3: continued from previous page

#	SMILES	Name	$\Delta G^{\mathrm{exp}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{hydr}}$	$\Delta G^{\mathrm{exp}}_{\mathrm{solv}}$	$\Delta G^{\mathrm{CG}}_{\mathrm{solv}}$
49	OCC=C	allyl alcohol	-5.11	-3.29	-5.35	-2.71
50	CS	methanethiol	-1.25	-2.20	-2.32	-2.75
51	OCC(F)(F)F	2,2,2-trifluoroethanol	-4.31	-2.16	-4.87	-2.72
52	CCCC	butane	2.08	1.88	-1.87	-1.49
53	CSC	dimethyl sulfide	-0.86	-1.15	-2.37	-2.08
54	CC(C)(C)O	2-methyl-2-propanol	-4.53	-2.22	-5.00	-2.74
55	CSSC	dimethyl disulfide	-1.85	-0.25	-4.27	-1.93
56	OCCO	1,2-ethanediol	-7.77	-4.40	-5.91	-2.38
57	CSC1=CC=CC=C1	thioanisole	-2.76	-6.15	-6.51	-11.11
58	c1ccsc1	thiophene	-1.42	-3.13	-3.90	-6.23
59	OC1=CC=CC=C1	phenol	-6.63	-7.70	-8.63	-11.30
60	C1=CC=NC=C1	pyridine	-4.70	-10.41	-5.59	-12.43
61	CC1=CC=C(O)C=C1	p-cresol	-6.15	-6.90	-8.81	-11.26
62	COC1=CC=CC=C1	anisole	-1.05	-6.89	-3.94	-11.06
63	C1=CN=CC=N1	pyrazine	-5.51	-15.75	-5.20	-13.87
64	CC(C)(C)C1=CC=C(O)C=C1	p-tert-butylphenol	-6.00	-10.10	-10.53	-16.00
65	N1C=CC=C1	pyrrole	-4.80	-6.35	-5.83	-7.74
66	COC	dimethyl ether	-1.90	-3.32	-2.04	-2.70
67	CC1=CNC2=CC=CC=C12	3-methylindole	-5.92	-12.96	-9.48	-16.87
68	CCOCC	diethyl ether	-1.60	-0.21	-2.82	-1.87
69	CCCCC	pentane	2.32	1.85	-2.31	-1.58