

Table S1 Compounds that failed the surface integration for at least one QM protocol.

key	index	charge	compound
140	0101pen	0	pentyl acetate
248	0221tri	0	triethylphosphate
249	0222tri	0	tripropylphosphate
145	0238met	0	methyl octanoate
253	0437pho	0	methyl 3-methyl-4-thiomethoxyphenyl thiophosphate
252	0438pho	0	diethyl 2,4-dichlorophenyl thiophosphate
251	0440pho	0	dimethyl 5-(4-chloro)bicyclo[3.2.0]heptyl phosphate
256	0441pho	0	dimethyl 4-nitrophenyl thiophosphate
259	0442pho	0	O-ethyl O'-4-bromo-2-chlorophenyl S-propyl phosphorothioate
254	0444pho	0	dimethyl 2,4,5-trichlorophenyl thiophosphate
255	0445pho	0	dimethyl 4-bromo-2,5-dichlorophenyl thiophosphate
257	0447pho	0	diethyl 4-nitrophenyl thiophosphonate
258	0449pho	0	ethyl 4-cyanophenyl phenylthiophosphonate
	i015	+1	tri-n-propylamine

Table S2 Compounds that required a nondefault surface integration origin for at least one QM protocol.

index	charge	compound	Integration origin (Å)			
			B3LYP/6-31+G*	HF/6-31+G*	HF/G3LARGE	B3LYP/G3LARGE
0007nhe	0	n-heptane			(-0.1 0.0 0.0)	
0008noc	0	n-octane			(-0.3 0.0 0.0)	
0037eth	0	ethylbenzene				center of mass
0058hep	0	1-heptanol	center of mass		center of mass	
0082hep	0	2-heptanone			center of mass	center of mass
0085non	0	5-nonanone	(-0.5 0.0 0.0)	center of mass	(0.0 0.2 0.0)	(-0.5 0.0 0.0)
0090hex	0	hexanoic acid	center of mass	center of mass	center of mass	center of mass
0099but	0	butyl acetate			(0.1 0.0 0.2)	
0100met	0	methyl hexanoate	center of mass	center of mass	center of mass	center of mass
0133nit	0	1-nitrobutane		center of mass		
0143dip	0	dipropyl sulfide			center of mass	
0236oct	0	1-octanol	center of mass	(-0.3 -0.1 -0.1)	(-0.3 -0.1 -0.1)	(-0.15 -0.1 0.0)
0237oct	0	octanal	center of mass	center of mass	(-0.3 -0.1 -0.1)	center of mass
0246eth	0	ethyl phenyl ether	center of mass	(0.4 0.0 0.0)	(0.0 0.0 -0.1)	
0401amia	0	1,1-dimethyl-3-phenylurea	(0.0 0.0 -0.5)		(0.0 0.0 -0.5)	(0.1 0.0 0.0)
0410clp	0	1-chloropentane		center of mass		
0419brt	0	bromotoluene				center of mass
0433pho	0	2,2-dichloroethenyl dimethyl phosphate	(-0.4 0.0 -0.2)	(-0.1 0.0 0.0)	(-0.1 0.0 -0.05)	(-0.1 0.0 0.0)
n013	0	N-ethylaniline	midpoint of outermost atoms	(0.4 0.0 0.0)	(0.4 0.0 0.0)	(0.4 0.0 0.0)
i012	+1	diallylamine	(0.0 -0.6 0.3)	(0.0 -0.6 0.3)	(0.0 -0.6 0.0)	(0.0 -0.6 0.0)
i024	+1	N-methylaniline	(-0.1 0.0 -0.5)			
i027	+1	4-methyl-N,N-dimethylaniline	(0.0 0.0 -0.5)	(-0.3 0.0 -0.5)		
i053	+1	diethyl ether				center of mass
i061	-1	hexanoic acid				center of mass

Empty boxes mean the default origin at the center of nuclear charge was satisfactory.

Table S 3-1

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/6-31+G* method for the cavity surface with constant density = 0.0005 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.14	2.14	-0.0012	0.0106	1.85	1.71	0.29
ethane	0	1.83	-0.13	1.96	-0.0015	0.0090	1.85	1.71	0.12
n-propane	0	1.96	-0.17	2.13	-0.0017	0.0090	1.85	1.68	0.28
n-butane	0	2.08	-0.20	2.28	-0.0017	0.0090	1.85	1.65	0.43
n-pentane	0	2.33	-0.23	2.56	-0.0018	0.0089	1.85	1.62	0.71
n-hexane	0	2.49	-0.26	2.75	-0.0019	0.0089	1.85	1.59	0.90
n-heptane	0	2.62	-0.29	2.91	-0.0019	0.0086	1.85	1.56	1.06
n-octane	0	2.89	-0.32	3.21	-0.0020	0.0085	1.85	1.53	1.36
2-methylpropane	0	2.32	-0.24	2.56	-0.0017	0.0090	1.85	1.60	0.72
2,2-dimethylpropane	0	2.50	-0.34	2.84	-0.0017	0.0091	1.85	1.51	0.99
2-methylpentane	0	2.52	-0.28	2.80	-0.0020	0.0090	1.85	1.57	0.95
2,4-dimethylpentane	0	2.88	-0.35	3.23	-0.0021	0.0096	1.85	1.49	1.39
2,2,4-trimethylpentane	0	2.85	-0.43	3.28	-0.0021	0.0106	1.85	1.42	1.43
cyclopropane	0	0.75	-0.73	1.48	-0.0098	0.0128	1.79	1.06	-0.31
cyclopentane	0	1.20	-0.20	1.40	-0.0020	0.0089	1.85	1.65	-0.45
cyclohexane	0	1.23	-0.17	1.40	-0.0020	0.0081	1.85	1.68	-0.45
methylcyclohexane	0	1.71	-0.23	1.94	-0.0019	0.0087	1.85	1.62	0.09
cis-1,2-dimethylcyclohexane	0	1.58	-0.27	1.85	-0.0020	0.0094	1.85	1.57	0.01
ethene	0	1.27	-1.03	2.30	-0.0112	0.0161	1.75	0.71	0.56
propene	0	1.27	-0.96	2.23	-0.0118	0.0149	1.73	0.77	0.50
1-butene	0	1.38	-0.91	2.29	-0.0121	0.0144	1.73	0.81	0.57
1-pentene	0	1.66	-0.94	2.60	-0.0121	0.0142	1.72	0.78	0.88
E-2-pentene	0	1.34	-0.79	2.13	-0.0117	0.0132	1.74	0.95	0.39
1-hexene	0	1.68	-1.03	2.71	-0.0120	0.0144	1.73	0.70	0.98
2-methylpropene	0	1.16	-0.96	2.12	-0.0124	0.0130	1.72	0.76	0.40
s-trans-1,3-butadiene	0	0.61	-1.78	2.39	-0.0100	0.0167	1.77	-0.01	0.62
cyclopentene	0	0.56	-0.75	1.31	-0.0121	0.0153	1.72	0.97	-0.41
ethyne	0	-0.01	-3.06	3.05	-0.0112	0.0384	1.45	-1.61	1.60
propyne	0	-0.31	-2.49	2.18	-0.0130	0.0355	1.47	-1.02	0.71
1-butyne	0	-0.16	-2.39	2.23	-0.0131	0.0354	1.46	-0.92	0.76
1-pentyne	0	0.01	-2.28	2.29	-0.0133	0.0351	1.46	-0.82	0.83
1-hexyne	0	0.29	-2.47	2.76	-0.0133	0.0350	1.46	-1.01	1.30

butenyne	0	0.04	-2.91	2.95	-0.0125	0.0377	1.43	-1.48	1.52
benzene	0	-0.87	-2.40	1.53	-0.0073	0.0178	1.81	-0.59	-0.28
ethylbenzene	0	-0.80	-2.26	1.46	-0.0082	0.0172	1.80	-0.46	-0.34
naphthalene	0	-2.39	-3.46	1.07	-0.0076	0.0183	1.80	-1.65	-0.74
anthracene	0	-4.23	-4.49	0.26	-0.0077	0.0188	1.80	-2.69	-1.54
toluene	0	-0.89	-2.26	1.37	-0.0083	0.0173	1.80	-0.46	-0.43
p-xylene	0	-0.81	-2.11	1.30	-0.0090	0.0159	1.79	-0.32	-0.49
m-xylene	0	-0.84	-2.13	1.29	-0.0091	0.0168	1.79	-0.34	-0.50
o-xylene	0	-0.90	-2.22	1.32	-0.0090	0.0165	1.79	-0.43	-0.47
fluoromethane	0	-0.22	-2.83	2.61	-0.0201	0.0184	1.18	-1.65	1.43
chloromethane	0	-0.56	-2.45	1.89	-0.0110	0.0212	1.73	-0.72	0.16
bromomethane	0	-0.82	-2.37	1.55	-0.0094	0.0219	1.76	-0.62	-0.20
chlorofluoromethane	0	-0.77	-3.66	2.89	-0.0132	0.0283	1.59	-2.07	1.30
dichloromethane	0	-1.36	-3.20	1.84	-0.0070	0.0299	1.70	-1.50	0.14
dibromomethane	0	-2.11	-3.14	1.03	-0.0058	0.0301	1.70	-1.44	-0.67
chlorodifluoromethane	0	-0.50	-3.20	2.70	-0.0081	0.0364	1.56	-1.64	1.14
chloroform	0	-1.07	-2.55	1.48	-0.0040	0.0366	1.58	-0.97	-0.10
chloroethane	0	-0.63	-2.41	1.78	-0.0117	0.0196	1.72	-0.70	0.07
bromoethane	0	-0.70	-2.36	1.66	-0.0101	0.0206	1.75	-0.61	-0.09
bromoform	0	-1.98	-2.82	0.84	-0.0035	0.0357	1.61	-1.21	-0.77
tetrafluoromethane	0	3.16	-0.97	4.13	-0.0028	0.0421	1.42	0.46	2.70
difluorodichloromethane	0	1.69	-0.78	2.47	-0.0039	0.0244	1.78	1.00	0.69
fluorotrichloromethane	0	0.82	-0.85	1.67	-0.0044	0.0230	1.79	0.94	-0.12
bromotrifluoromethane	0	1.79	-1.04	2.83	-0.0037	0.0410	1.46	0.42	1.37
bromotrichloromethane	0	-0.93	-1.21	0.28	-0.0020	0.0308	1.70	0.49	-1.42
hexafluoroethane	0	3.94	-0.94	4.88	-0.0028	0.0417	1.44	0.50	3.44
hexachloroethane	0	-1.40	-1.35	-0.05	-0.0030	0.0222	1.80	0.45	-1.85
chloropentafluoroethane	0	2.86	-0.89	3.75	-0.0037	0.0395	1.51	0.61	2.25
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.06	2.83	-0.0054	0.0235	1.78	0.72	1.05
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-3.40	3.92	-0.0087	0.0383	1.50	-1.89	2.41
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-3.05	2.92	-0.0059	0.0380	1.54	-1.51	1.38
1-chloro-2,2,2-trifluoroethane	0	0.06	-3.60	3.66	-0.0075	0.0337	1.63	-1.97	2.03
1,1,1,2-tetrachloroethane	0	-1.15	-2.92	1.77	-0.0069	0.0299	1.70	-1.22	0.07
1,1,1-trichloroethane	0	-0.25	-2.01	1.76	-0.0050	0.0215	1.80	-0.21	-0.04
1,1,2-trichloroethane	0	-1.95	-3.70	1.75	-0.0075	0.0318	1.66	-2.04	0.09

1,1-difluoroethane	0	-0.11	-3.55	3.44	-0.0155	0.0238	1.53	-2.02	1.91
1-bromo-2-chloroethane	0	-1.95	-3.21	1.26	-0.0088	0.0244	1.74	-1.47	-0.48
octafluoropropane	0	4.28	-1.07	5.35	-0.0028	0.0413	1.45	0.38	3.90
2-chloropropane	0	-0.25	-2.36	2.11	-0.0122	0.0185	1.70	-0.66	0.41
1-chloropropane	0	-0.27	-2.37	2.10	-0.0117	0.0190	1.72	-0.65	0.38
1-bromopropane	0	-0.56	-2.34	1.78	-0.0102	0.0200	1.75	-0.59	0.03
2-bromopropane	0	-0.48	-2.32	1.84	-0.0106	0.0196	1.75	-0.58	0.10
2-chlorobutane	0	0.07	-2.22	2.29	-0.0125	0.0182	1.70	-0.52	0.59
1-bromobutane	0	-0.41	-2.37	1.96	-0.0102	0.0200	1.75	-0.62	0.21
1-chloropentane	0	0.07	-2.43	2.50	-0.0118	0.0189	1.72	-0.72	0.79
2-chloropentane	0	0.07	-2.21	2.28	-0.0124	0.0179	1.70	-0.51	0.58
1-bromopentane	0	-0.08	-2.40	2.32	-0.0103	0.0200	1.75	-0.65	0.57
1-bromo-isobutane	0	-0.03	-2.21	2.18	-0.0102	0.0201	1.75	-0.46	0.43
tetrachloroethene	0	0.05	-1.10	1.15	-0.0035	0.0216	1.80	0.70	-0.65
trichloroethene	0	-0.39	-1.90	1.51	-0.0052	0.0340	1.64	-0.26	-0.13
chloroethene	0	-0.59	-2.06	1.47	-0.0087	0.0259	1.73	-0.33	-0.26
E-1,2-dichloroethene	0	-0.76	-2.15	1.39	-0.0059	0.0304	1.70	-0.45	-0.31
Z-1,2-dichloroethene	0	-1.17	-2.92	1.75	-0.0072	0.0310	1.68	-1.24	0.07
3-chloropropene	0	-0.57	-2.72	2.15	-0.0107	0.0213	1.73	-0.99	0.42
3-bromopropene	0	-0.86	-3.07	2.21	-0.0100	0.0226	1.74	-1.33	0.47
fluorobenzene	0	-0.78	-2.91	2.13	-0.0156	0.0217	1.54	-1.37	0.59
chlorobenzene	0	-1.12	-2.69	1.57	-0.0083	0.0218	1.77	-0.92	-0.20
bromobenzene	0	-1.46	-2.75	1.29	-0.0072	0.0219	1.78	-0.96	-0.50
1,4-dichlorobenzene	0	-1.01	-2.74	1.73	-0.0069	0.0250	1.76	-0.98	-0.03
1,2-dichlorobenzene	0	-1.36	-3.00	1.64	-0.0084	0.0245	1.75	-1.25	-0.11
p-dibromobenzene	0	-2.30	-2.83	0.53	-0.0059	0.0248	1.77	-1.06	-1.24
chlorotoluene	0	-1.92	-4.37	2.45	-0.0119	0.0218	1.70	-2.67	0.75
o-chlorotoluene	0	-1.15	-2.42	1.27	-0.0086	0.0215	1.77	-0.65	-0.50
bromotoluene	0	-2.37	-4.34	1.97	-0.0103	0.0229	1.73	-2.61	0.24
p-bromotoluene	0	-1.39	-2.68	1.29	-0.0077	0.0216	1.78	-0.90	-0.49
2,3-dichlorobiphenyl	0	-2.45	-4.24	1.79	-0.0089	0.0240	1.75	-2.49	0.04
2,2'-dichlorobiphenyl	0	-2.73	-4.63	1.90	-0.0093	0.0219	1.76	-2.87	0.14
2,2',3'-trichlorobiphenyl	0	-1.99	-4.49	2.50	-0.0090	0.0244	1.74	-2.75	0.76
1,2-dimethoxyethane	0	-4.84	-3.64	-1.20	-0.0268	0.0132	0.13	-3.51	-1.33
anisole	0	-2.45	-3.77	1.32	-0.0242	0.0193	0.62	-3.15	0.70

dimethyl ether	0	-1.92	-2.63	0.71	-0.0283	0.0131	-0.21	-2.84	0.92
diethyl ether	0	-1.76	-2.53	0.77	-0.0290	0.0121	-0.38	-2.91	1.15
isopropyl ether	0	-0.53	-2.28	1.75	-0.0289	0.0125	-0.36	-2.64	2.11
methyl propyl ether	0	-1.66	-2.37	0.71	-0.0281	0.0125	-0.15	-2.52	0.86
methyl isopropyl ether	0	-2.01	-2.33	0.32	-0.0282	0.0121	-0.19	-2.52	0.51
t-butyl methyl ether	0	-2.21	-2.27	0.06	-0.0283	0.0120	-0.21	-2.49	0.28
ethyl phenyl ether	0	-2.22	-3.58	1.36	-0.0241	0.0191	0.63	-2.95	0.73
tetrahydrofuran	0	-3.47	-2.95	-0.52	-0.0298	0.0130	-0.61	-3.56	0.09
tetrahydropyran	0	-3.12	-2.60	-0.52	-0.0293	0.0116	-0.46	-3.06	-0.06
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-4.32	4.20	-0.0180	0.0307	1.26	-3.06	2.94
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-5.08	5.19	-0.0119	0.0381	1.44	-3.64	3.75
acetaldehyde	0	-3.50	-5.33	1.83	-0.0280	0.0232	-0.19	-5.52	2.02
propanal	0	-3.44	-4.94	1.50	-0.0283	0.0224	-0.25	-5.19	1.75
butanal	0	-3.18	-5.10	1.92	-0.0281	0.0224	-0.22	-5.32	2.14
pentanal	0	-3.03	-4.97	1.94	-0.0283	0.0222	-0.24	-5.22	2.19
octanal	0	-2.29	-5.07	2.78	-0.0281	0.0218	-0.21	-5.28	2.99
benzaldehyde	0	-4.02	-6.02	2.00	-0.0287	0.0237	-0.36	-6.38	2.36
p-hydroxybenzaldehyde	0	-10.48	-10.37	-0.11	-0.0296	0.0695	-2.90	-13.27	2.79
m-hydroxybenzaldehyde	0	-9.51	-9.84	0.33	-0.0283	0.0688	-2.46	-12.30	2.79
acetone	0	-3.85	-5.43	1.58	-0.0292	0.0217	-0.47	-5.90	2.05
2-butanone	0	-3.64	-5.02	1.38	-0.0294	0.0210	-0.52	-5.54	1.90
2-pentanone	0	-3.53	-5.01	1.48	-0.0295	0.0211	-0.55	-5.56	2.03
3-pentanone	0	-3.41	-4.60	1.19	-0.0289	0.0206	-0.39	-4.99	1.58
2-hexanone	0	-3.29	-5.05	1.76	-0.0294	0.0209	-0.54	-5.60	2.31
2-heptanone	0	-3.04	-5.08	2.04	-0.0295	0.0209	-0.57	-5.65	2.61
4-heptanone	0	-2.93	-4.60	1.67	-0.0289	0.0203	-0.39	-4.99	2.06
2-octanone	0	-2.88	-5.10	2.22	-0.0295	0.0206	-0.56	-5.66	2.78
5-nonanone	0	-2.67	-4.68	2.01	-0.0290	0.0203	-0.41	-5.09	2.42
3,3-dimethylbutanone	0	-2.89	-4.68	1.79	-0.0294	0.0185	-0.53	-5.21	2.32
cyclopentanone	0	-4.68	-5.45	0.77	-0.0294	0.0208	-0.54	-5.99	1.31
acetophenone	0	-4.58	-5.93	1.35	-0.0297	0.0221	-0.62	-6.54	1.96
methyl formate	0	-2.78	-5.04	2.26	-0.0264	0.0276	0.12	-4.93	2.15
ethyl formate	0	-2.65	-4.93	2.28	-0.0267	0.0271	0.07	-4.86	2.21
methyl acetate	0	-3.32	-4.75	1.43	-0.0279	0.0242	-0.16	-4.92	1.60
ethyl acetate	0	-3.10	-4.69	1.59	-0.0281	0.0237	-0.22	-4.90	1.80

propyl acetate	0	-2.86	-4.69	1.83	-0.0281	0.0231	-0.22	-4.91	2.05
butyl acetate	0	-2.55	-4.72	2.17	-0.0281	0.0225	-0.21	-4.93	2.38
methyl propanoate	0	-2.93	-4.46	1.53	-0.0275	0.0237	-0.08	-4.54	1.61
methyl butanoate	0	-2.83	-4.48	1.65	-0.0277	0.0236	-0.11	-4.59	1.76
methyl pentanoate	0	-2.57	-4.51	1.94	-0.0277	0.0232	-0.12	-4.63	2.06
methyl hexanoate	0	-2.49	-4.53	2.04	-0.0277	0.0230	-0.12	-4.65	2.16
methyl benzoate	0	-3.91	-5.07	1.16	-0.0277	0.0215	-0.11	-5.18	1.27
hydrogen	0	2.33	-0.07	2.40	-0.0006	0.0096	1.85	1.78	0.55
water	0	-6.31	-7.45	1.14	-0.0287	0.0589	-1.65	-9.10	2.79
water dimer	0	-11.27	-11.67	0.40	-0.0324	0.0664	-3.41	-15.07	3.80
hydrogen peroxide	0	-8.58	-8.21	-0.37	-0.0232	0.0673	-1.30	-9.51	0.93
methyl peroxide	0	-5.28	-6.08	0.80	-0.0240	0.0664	-1.34	-7.42	2.14
ethyl peroxide	0	-5.32	-6.01	0.69	-0.0244	0.0655	-1.31	-7.32	2.00
1,4-dioxane	0	-5.05	-4.46	-0.59	-0.0275	0.0156	-0.04	-4.49	-0.56
methanol	0	-5.11	-5.02	-0.09	-0.0288	0.0562	-1.46	-6.48	1.37
ethanol	0	-5.01	-4.66	-0.35	-0.0286	0.0559	-1.39	-6.05	1.04
1-propanol	0	-4.83	-4.63	-0.20	-0.0286	0.0550	-1.33	-5.97	1.14
isopropanol	0	-4.76	-4.45	-0.31	-0.0292	0.0513	-1.27	-5.73	0.97
1-butanol	0	-4.72	-4.67	-0.05	-0.0286	0.0547	-1.32	-5.99	1.27
t-butanol	0	-4.51	-4.20	-0.31	-0.0289	0.0513	-1.18	-5.38	0.87
1-pentanol	0	-4.47	-4.80	0.33	-0.0291	0.0531	-1.35	-6.15	1.68
1-hexanol	0	-4.36	-4.82	0.46	-0.0293	0.0528	-1.37	-6.19	1.83
1-heptanol	0	-4.24	-4.83	0.59	-0.0293	0.0522	-1.34	-6.17	1.93
1-octanol	0	-4.09	-4.88	0.79	-0.0291	0.0523	-1.30	-6.18	2.09
allyl alcohol	0	-5.08	-4.76	-0.32	-0.0286	0.0543	-1.29	-6.05	0.97
cyclopentanol	0	-5.49	-4.20	-1.29	-0.0294	0.0492	-1.20	-5.40	-0.09
2-methoxyethanol	0	-6.77	-6.48	-0.29	-0.0280	0.0570	-1.32	-7.80	1.03
2,2,2-trifluoroethanol	0	-4.31	-7.94	3.63	-0.0224	0.0682	-1.27	-9.22	4.91
1,1,1-trifluoropropan-2-ol	0	-4.16	-5.19	1.03	-0.0245	0.0612	-0.94	-6.13	1.97
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-5.80	2.03	-0.0194	0.0722	-1.38	-7.18	3.41
phenol	0	-6.62	-6.29	-0.33	-0.0238	0.0648	-1.13	-7.42	0.80
p-bromophenol	0	-7.13	-6.79	-0.34	-0.0222	0.0661	-1.02	-7.81	0.68
o-cresol	0	-5.87	-5.72	-0.15	-0.0231	0.0642	-0.97	-6.69	0.82
m-cresol	0	-5.49	-6.14	0.65	-0.0241	0.0645	-1.15	-7.29	1.80
p-cresol	0	-6.14	-6.10	-0.04	-0.0243	0.0639	-1.14	-7.24	1.10

1,2-ethanediol	0	-9.30	-8.10	-1.20	-0.0302	0.0617	-2.29	-10.39	1.09
acetic acid	0	-6.70	-6.92	0.22	-0.0271	0.0713	-2.48	-9.40	2.70
propanoic acid	0	-6.47	-6.61	0.14	-0.0268	0.0711	-2.39	-9.00	2.53
butanoic acid	0	-6.36	-6.61	0.25	-0.0268	0.0707	-2.36	-8.97	2.61
pentanoic acid	0	-6.16	-6.65	0.49	-0.0267	0.0708	-2.34	-8.99	2.83
hexanoic acid	0	-6.21	-6.68	0.47	-0.0269	0.0709	-2.38	-9.06	2.85
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-11.41	-0.55	-0.0237	0.0748	-2.29	-13.69	1.73
ammonia	0	-4.29	-4.51	0.22	-0.0315	0.0315	-1.28	-5.80	1.51
methylamine	0	-4.56	-3.42	-1.14	-0.0307	0.0301	-1.00	-4.42	-0.14
ethylamine	0	-4.50	-3.46	-1.04	-0.0308	0.0292	-1.03	-4.49	-0.01
butylamine	0	-4.29	-3.49	-0.80	-0.0310	0.0290	-1.06	-4.55	0.26
propylamine	0	-4.39	-3.47	-0.92	-0.0309	0.0292	-1.06	-4.53	0.14
pentylamine	0	-4.10	-3.51	-0.59	-0.0311	0.0286	-1.09	-4.60	0.50
dimethylamine	0	-4.29	-2.43	-1.86	-0.0294	0.0297	-0.62	-3.05	-1.24
diethylamine	0	-4.07	-2.30	-1.77	-0.0291	0.0280	-0.52	-2.82	-1.25
dipropylamine	0	-3.66	-2.33	-1.33	-0.0289	0.0278	-0.47	-2.80	-0.86
trimethylamine	0	-3.23	-1.52	-1.71	-0.0278	0.0110	-0.09	-1.61	-1.62
azetidine	0	-5.56	-2.77	-2.79	-0.0307	0.0293	-0.98	-3.75	-1.81
pyrrolidine	0	-5.48	-2.94	-2.54	-0.0306	0.0284	-0.94	-3.88	-1.60
piperidine	0	-5.11	-2.04	-3.07	-0.0288	0.0294	-0.46	-2.49	-2.62
2-methoxyethanamine	0	-6.55	-5.61	-0.94	-0.0300	0.0313	-0.83	-6.43	-0.12
1,2-ethanediamine	0	-9.72	-6.73	-2.99	-0.0301	0.0309	-0.83	-7.56	-2.16
nitromethane	0	-3.95	-7.15	3.20	-0.0220	0.0299	0.85	-6.30	2.35
nitroethane	0	-3.71	-6.68	2.97	-0.0226	0.0284	0.78	-5.90	2.19
1-nitropropane	0	-3.34	-6.53	3.19	-0.0226	0.0279	0.79	-5.74	2.40
2-nitropropane	0	-3.14	-6.02	2.88	-0.0230	0.0271	0.74	-5.29	2.15
1-nitrobutane	0	-3.08	-6.54	3.46	-0.0227	0.0277	0.78	-5.76	2.68
nitrobenzene	0	-4.12	-6.00	1.88	-0.0220	0.0269	0.88	-5.12	1.00
2-methyl-1-nitrobenzene	0	-3.59	-5.62	2.03	-0.0230	0.0253	0.77	-4.86	1.27
pyridine	0	-4.70	-4.05	-0.65	-0.0293	0.0235	-0.53	-4.59	-0.11
2-methylpyridine	0	-4.63	-3.62	-1.01	-0.0293	0.0224	-0.51	-4.13	-0.50
3-methylpyridine	0	-4.77	-3.99	-0.78	-0.0297	0.0220	-0.63	-4.62	-0.15
4-methylpyridine	0	-4.94	-4.10	-0.84	-0.0301	0.0201	-0.71	-4.81	-0.13
4-ethylpyridine	0	-4.74	-4.06	-0.68	-0.0301	0.0201	-0.71	-4.78	0.04
2,4-dimethylpyridine	0	-4.86	-3.67	-1.19	-0.0299	0.0190	-0.67	-4.33	-0.53

2,5-dimethylpyridine	0	-4.72	-3.55	-1.17	-0.0295	0.0212	-0.56	-4.12	-0.60
2,6-dimethylpyridine	0	-4.60	-3.22	-1.38	-0.0291	0.0219	-0.46	-3.68	-0.92
3,4-dimethylpyridine	0	-5.22	-4.13	-1.09	-0.0303	0.0198	-0.78	-4.91	-0.31
3,5-dimethylpyridine	0	-4.84	-3.94	-0.90	-0.0300	0.0209	-0.71	-4.65	-0.19
aniline	0	-5.49	-5.61	0.12	-0.0247	0.0403	0.19	-5.42	-0.07
N-methylaniline	0	-4.68	-4.44	-0.24	-0.0219	0.0400	0.64	-3.80	-0.88
2-methylaniline	0	-5.56	-5.07	-0.49	-0.0249	0.0389	0.20	-4.87	-0.69
3-methylaniline	0	-5.67	-5.44	-0.23	-0.0248	0.0393	0.20	-5.24	-0.43
4-methylaniline	0	-5.55	-5.39	-0.16	-0.0253	0.0388	0.12	-5.26	-0.29
N-ethylaniline	0	-4.62	-4.27	-0.35	-0.0197	0.0409	0.87	-3.41	-1.21
3-aminoaniline	0	-9.92	-8.84	-1.08	-0.0247	0.0399	0.21	-8.63	-1.29
N,N-dimethylaniline	0	-3.58	-3.32	-0.26	-0.0183	0.0165	1.37	-1.96	-1.62
piperazine	0	-7.40	-3.82	-3.58	-0.0286	0.0300	-0.41	-4.23	-3.17
N-methylpiperazine	0	-7.77	-3.03	-4.74	-0.0285	0.0304	-0.41	-3.44	-4.33
N,N'-dimethylpiperazine	0	-7.58	-2.21	-5.37	-0.0269	0.0113	0.13	-2.08	-5.50
1-methylthymine	0	-10.40	-11.61	1.21	-0.0301	0.0610	-2.18	-13.79	3.39
9-methyladenine	0	-13.60	-9.34	-4.26	-0.0282	0.0500	-0.95	-10.28	-3.32
acetamide	0	-9.71	-9.08	-0.63	-0.0318	0.0517	-2.06	-11.14	1.43
E-N-methylacetamide	0	-10.00	-8.09	-1.91	-0.0330	0.0460	-2.20	-10.29	0.29
Z-N-methylacetamide	0	-10.00	-7.68	-2.32	-0.0331	0.0513	-2.49	-10.16	0.16
benzamide	0	-10.90	-9.10	-1.80	-0.0309	0.0504	-1.71	-10.80	-0.10
2,6-dichlorothiobenzamide	0	-10.81	-10.82	0.01	-0.0197	0.0629	-0.42	-11.24	0.43
urea	0	-13.80	-11.09	-2.71	-0.0309	0.0502	-1.70	-12.79	-1.01
1,1-dimethyl-3-phenylurea	0	-9.63	-8.57	-1.06	-0.0302	0.0484	-1.41	-9.97	0.34
hydrazine	0	-6.26	-5.60	-0.66	-0.0286	0.0322	-0.45	-6.05	-0.21
methylhydrazine	0	-5.31	-5.26	-0.05	-0.0288	0.0324	-0.51	-5.77	0.46
1,1-dimethylhydrazine	0	-4.48	-4.16	-0.32	-0.0288	0.0324	-0.52	-4.67	0.19
2-methylpyrazine	0	-5.57	-3.98	-1.59	-0.0260	0.0225	0.26	-3.73	-1.84
2-ethylpyrazine	0	-5.51	-3.68	-1.83	-0.0261	0.0223	0.24	-3.44	-2.07
morpholine	0	-7.17	-4.28	-2.89	-0.0289	0.0322	-0.53	-4.81	-2.36
N-methylmorpholine	0	-6.34	-3.38	-2.96	-0.0287	0.0134	-0.31	-3.69	-2.65
acetonitrile	0	-3.89	-6.00	2.11	-0.0257	0.0257	0.30	-5.70	1.81
butanonitrile	0	-3.64	-5.46	1.82	-0.0258	0.0235	0.29	-5.16	1.52
propionitrile	0	-3.85	-5.67	1.82	-0.0258	0.0234	0.28	-5.38	1.53
benzonitrile	0	-4.10	-6.07	1.97	-0.0253	0.0266	0.36	-5.71	1.61

2,6-dichlorobenzonitrile	0	-5.22	-6.40	1.18	-0.0242	0.0298	0.51	-5.90	0.68
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-7.87	-1.13	-0.0238	0.0580	-0.55	-8.42	-0.58
trimethylphosphate	0	-8.70	-8.40	-0.30	-0.0316	0.0276	-1.24	-9.64	0.94
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-7.54	0.93	-0.0281	0.0340	-0.37	-7.91	1.30
phosphine	0	0.60	-0.67	1.27	-0.0118	0.0171	1.73	1.06	-0.46
hydrogen sulfide	0	-0.70	-2.11	1.41	-0.0131	0.0207	1.66	-0.45	-0.25
dimethyl sulfide	0	-1.54	-2.25	0.71	-0.0164	0.0165	1.51	-0.74	-0.80
diethyl sulfide	0	-1.43	-2.06	0.63	-0.0169	0.0132	1.48	-0.58	-0.85
dipropyl sulfide	0	-1.27	-2.14	0.87	-0.0171	0.0128	1.47	-0.66	-0.61
bis(2-chloroethyl)sulfide	0	-3.92	-4.85	0.93	-0.0121	0.0220	1.69	-3.16	-0.76
dimethyl disulfide	0	-1.83	-2.83	1.00	-0.0136	0.0190	1.65	-1.18	-0.65
diethyl disulfide	0	-1.63	-2.50	0.87	-0.0141	0.0173	1.64	-0.86	-0.77
methanethiol	0	-1.24	-2.21	0.97	-0.0151	0.0178	1.58	-0.63	-0.61
ethanethiol	0	-1.30	-2.15	0.85	-0.0153	0.0165	1.58	-0.57	-0.73
1-propanethiol	0	-1.05	-2.18	1.13	-0.0153	0.0163	1.58	-0.60	-0.45
thiophene	0	-1.42	-2.69	1.27	-0.0086	0.0251	1.74	-0.95	-0.47
thiophenol	0	-2.55	-3.66	1.11	-0.0126	0.0211	1.68	-1.99	-0.56
thioanisole	0	-2.73	-3.73	1.00	-0.0141	0.0195	1.63	-2.11	-0.62
tetramethylsilane	0	3.04	-0.76	3.80	-0.0053	0.0103	1.84	1.08	1.96
acetylene	-1	-76.50	-62.00	-14.50	-0.0477	0.0061	-10.32	-72.32	-4.18
acetonitrile	-1	-66.60	-57.56	-9.04	-0.0472	-0.0053	-9.84	-67.40	0.80
cyanamide	-1	-72.20	-61.55	-10.65	-0.0475	0.0103	-10.12	-71.67	-0.53
aniline	-1	-62.90	-53.58	-9.32	-0.0508	0.0042	-13.16	-66.74	3.84
diphenylamine	-1	-54.60	-47.23	-7.37	-0.0446	0.0071	-7.80	-55.04	0.44
hydrogen cyanide	-1	-70.20	-63.09	-7.11	-0.0477	-0.0335	-10.26	-73.34	3.14
formic acid	-1	-76.20	-64.05	-12.15	-0.0503	-0.0079	-12.67	-76.72	0.52
acetic acid	-1	-77.60	-63.32	-14.28	-0.0513	0.0005	-13.72	-77.04	-0.56
propanoic acid	-1	-76.20	-61.50	-14.70	-0.0513	0.0026	-13.73	-75.23	-0.97
hexanoic acid	-1	-74.60	-60.70	-13.90	-0.0513	0.0082	-13.71	-74.41	-0.19
acrylic acid	-1	-74.00	-62.04	-11.96	-0.0510	0.0088	-13.43	-75.47	1.47
pyruvic acid	-1	-68.50	-60.98	-7.52	-0.0485	0.0137	-11.02	-72.00	3.50
benzoic acid	-1	-71.20	-59.51	-11.69	-0.0504	0.0127	-12.80	-72.31	1.11
methanol	-1	-95.00	-66.31	-28.69	-0.0606	-0.0189	-25.50	-91.81	-3.19
ethanol	-1	-90.70	-63.27	-27.43	-0.0604	-0.0051	-25.29	-88.56	-2.14
1-propanol	-1	-88.30	-62.42	-25.88	-0.0605	0.0005	-25.34	-87.76	-0.54

isopropanol	-1	-86.30	-60.49	-25.81	-0.0601	-0.0048	-24.73	-85.22	-1.08
2-butanol	-1	-84.20	-57.62	-26.58	-0.0594	-0.0043	-23.67	-81.29	-2.91
t-butanol	-1	-82.30	-58.05	-24.25	-0.0597	-0.0043	-24.21	-82.26	-0.04
allyl alcohol	-1	-86.60	-62.00	-24.60	-0.0599	0.0025	-24.53	-86.52	-0.08
benzyl alcohol	-1	-85.10	-58.28	-26.82	-0.0586	0.0093	-22.51	-80.79	-4.31
2-methoxyethanol	-1	-89.40	-63.66	-25.74	-0.0601	0.0054	-24.72	-88.38	-1.02
phenol	-1	-71.90	-55.95	-15.95	-0.0529	0.0049	-15.39	-71.34	-0.56
2-methylphenol	-1	-70.20	-54.09	-16.11	-0.0529	0.0039	-15.38	-69.46	-0.74
3-methylphenol	-1	-71.10	-55.77	-15.33	-0.0531	0.0055	-15.58	-71.35	0.25
4-methylphenol	-1	-72.00	-55.82	-16.18	-0.0535	0.0043	-16.04	-71.86	-0.14
1,2-ethanediol	-1	-85.30	-66.25	-19.05	-0.0601	0.0439	-25.30	-91.55	6.25
3-hydroxyphenol	-1	-73.80	-57.36	-16.44	-0.0519	0.0523	-15.17	-72.53	-1.27
4-hydroxyphenol	-1	-77.60	-59.08	-18.52	-0.0535	0.0497	-16.84	-75.92	-1.68
methyl hydroperoxide	-1	-93.20	-68.10	-25.10	-0.0575	-0.0044	-21.08	-89.18	-4.02
ethyl hydroperoxide	-1	-89.20	-67.00	-22.20	-0.0576	0.0029	-21.19	-88.19	-1.01
acetaldehyde	-1	-76.50	-60.38	-16.12	-0.0542	-0.0062	-16.82	-77.21	0.71
acetone	-1	-76.20	-59.07	-17.13	-0.0544	-0.0015	-17.08	-76.15	-0.05
3-pentanone	-1	-73.70	-54.44	-19.26	-0.0537	0.0001	-16.28	-70.72	-2.98
water	-1	-104.70	-74.86	-29.84	-0.0637	-0.0073	-30.51	-105.37	0.67
hydrogen peroxide	-1	-97.30	-72.74	-24.56	-0.0576	0.0230	-21.25	-93.99	-3.31
hydroperoxyl radical	-1	-83.30	-69.71	-13.59	-0.0517	-0.0440	-14.13	-83.84	0.54
2-nitrophenol	-1	-60.10	-54.07	-6.03	-0.0475	0.0123	-10.14	-64.21	4.11
3-nitrophenol	-1	-61.90	-50.77	-11.13	-0.0496	0.0175	-11.99	-62.76	0.86
4-nitrophenol	-1	-57.80	-49.10	-8.70	-0.0456	0.0136	-8.56	-57.65	-0.15
nitromethane	-1	-76.50	-61.86	-14.64	-0.0493	0.0039	-11.71	-73.56	-2.94
4-nitroaniline	-1	-57.40	-48.50	-8.90	-0.0434	0.0125	-6.93	-55.43	-1.97
acetamide	-1	-80.20	-60.32	-19.88	-0.0515	-0.0009	-13.87	-74.20	-6.00
methanethiol	-1	-73.80	-58.34	-15.46	-0.0392	-0.0050	-4.38	-62.72	-11.08
ethanethiol	-1	-71.80	-56.44	-15.36	-0.0391	-0.0015	-4.30	-60.74	-11.06
1-propanethiol	-1	-70.50	-56.04	-14.46	-0.0391	0.0037	-4.32	-60.36	-10.14
thiophenol	-1	-63.40	-52.95	-10.45	-0.0359	0.0089	-2.75	-55.70	-7.70
hydrogen sulfide	-1	-72.10	-59.77	-12.33	-0.0389	-0.0131	-4.23	-64.00	-8.10
dimethyl sulfoxide	-1	-67.70	-57.52	-10.18	-0.0520	0.0046	-14.37	-71.89	4.19
hydrofluoric acid	-1	-104.40	-80.55	-23.85	-0.0656	-0.0656	-34.08	-114.63	10.23
hydrochloric acid	-1	-74.50	-63.88	-10.62	-0.0404	-0.0404	-5.02	-68.90	-5.60

hydrobromic acid	-1	-68.30	-60.03	-8.27	-0.0353	-0.0353	-2.49	-62.52	-5.78
chloroform	-1	-54.10	-49.27	-4.83	-0.0355	-0.0116	-2.61	-51.88	-2.22
trifluoroacetic acid	-1	-59.30	-56.49	-2.81	-0.0456	0.0245	-8.66	-65.15	5.85
chloroacetic acid	-1	-69.70	-58.61	-11.09	-0.0480	0.0095	-10.55	-69.15	-0.55
dichloroacetic acid	-1	-62.30	-55.22	-7.08	-0.0456	0.0152	-8.60	-63.82	1.52
2,2,2-trifluoroethanol	-1	-77.50	-59.37	-18.13	-0.0566	0.0049	-19.87	-79.24	1.74
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-54.58	-10.92	-0.0529	0.0114	-15.36	-69.94	4.44
2-chlorophenol	-1	-66.10	-53.80	-12.30	-0.0508	0.0095	-13.19	-66.99	0.89
4-chlorophenol	-1	-66.00	-52.14	-13.86	-0.0512	0.0095	-13.61	-65.74	-0.26
methylamine	1	-76.40	-70.46	-5.94	0.0239	0.0889	-3.57	-74.03	-2.37
n-propylamine	1	-71.50	-65.71	-5.79	0.0061	0.0885	-3.48	-69.19	-2.31
isopropylamine	1	-69.60	-64.00	-5.60	0.0107	0.0861	-3.01	-67.01	-2.59
tert-butylamine	1	-67.30	-61.35	-5.95	0.0106	0.0844	-2.69	-64.05	-3.25
cyclohexanamine	1	-68.70	-61.16	-7.54	0.0064	0.0855	-2.89	-64.05	-4.65
allylamine	1	-72.00	-65.60	-6.40	-0.0025	0.0889	-3.57	-69.17	-2.83
dimethylamine	1	-68.60	-63.07	-5.53	0.0215	0.0838	-2.58	-65.65	-2.95
diethylamine	1	-63.40	-57.26	-6.14	0.0104	0.0786	-1.71	-58.97	-4.43
di-n-propylamine	1	-60.50	-55.13	-5.37	0.0067	0.0784	-1.68	-56.81	-3.69
diallylamine	1	-61.60	-55.31	-6.29	-0.0018	0.0800	-1.93	-57.25	-4.35
trimethylamine	1	-61.10	-56.81	-4.29	0.0207	0.0795	-1.85	-58.66	-2.44
triethylamine	1	-54.60	-49.49	-5.11	0.0092	0.0688	-0.42	-49.91	-4.69
aniline	1	-72.40	-65.37	-7.03	0.0002	0.0920	-4.22	-69.60	-2.80
2-methylaniline	1	-70.30	-63.03	-7.27	-0.0005	0.0905	-3.91	-66.95	-3.35
3-methylaniline	1	-69.60	-63.86	-5.74	-0.0009	0.0911	-4.03	-67.90	-1.70
4-methylaniline	1	-69.80	-63.67	-6.13	-0.0002	0.0906	-3.92	-67.60	-2.20
3-aminoaniline	1	-65.80	-65.87	0.07	-0.0146	0.0908	-4.20	-70.06	4.26
N-methylaniline	1	-62.60	-58.14	-4.46	-0.0003	0.0854	-2.87	-61.02	-1.58
N-ethylaniline	1	-62.20	-55.37	-6.83	-0.0004	0.0826	-2.37	-57.74	-4.46
N,N-dimethylaniline	1	-57.20	-52.09	-5.11	-0.0004	0.0790	-1.78	-53.87	-3.33
4-methyl-N,N-dimethylaniline	1	-55.90	-50.73	-5.17	-0.0007	0.0781	-1.63	-52.36	-3.54
N,N-diethylaniline	1	-54.00	-48.04	-5.96	-0.0016	0.0730	-0.92	-48.96	-5.04
1-aminonaphthalene	1	-67.40	-62.24	-5.16	-0.0020	0.0928	-4.41	-66.65	-0.75
aziridine	1	-70.90	-64.61	-6.29	0.0233	0.0891	-3.60	-68.21	-2.69
azetidine	1	-67.70	-61.02	-6.68	0.0161	0.0835	-2.53	-63.55	-4.15
pyrrolidine	1	-66.00	-59.07	-6.93	0.0118	0.0828	-2.40	-61.47	-4.53

piperidine	1	-64.20	-57.30	-6.90	0.0107	0.0827	-2.39	-59.69	-4.51
azacycloheptane	1	-63.30	-55.76	-7.54	0.0094	0.0829	-2.42	-58.18	-5.12
pyrrole	1	-61.40	-57.57	-3.83	0.0104	0.0885	-3.48	-61.05	-0.35
pyridine	1	-61.10	-56.26	-4.84	0.0125	0.0917	-4.17	-60.42	-0.68
quinoline	1	-56.00	-50.96	-5.04	0.0028	0.0855	-2.90	-53.86	-2.14
piperazine	1	-66.00	-59.25	-6.75	-0.0174	0.0832	-2.86	-62.11	-3.89
acetonitrile	1	-75.30	-65.15	-10.15	0.0275	0.1233	-14.63	-79.78	4.48
ammonia	1	-85.20	-79.80	-5.40	0.0493	0.0950	-4.94	-84.74	-0.46
hydrazine	1	-84.60	-77.78	-6.82	-0.0072	0.0930	-4.49	-82.27	-2.33
methanol	1	-93.00	-77.16	-15.84	0.0126	0.1309	-18.35	-95.51	2.51
ethanol	1	-88.40	-72.02	-16.38	0.0099	0.1290	-17.33	-89.35	0.95
dimethyl ether	1	-79.70	-64.76	-14.94	0.0096	0.1223	-14.16	-78.92	-0.78
diethyl ether	1	-71.50	-57.29	-14.21	0.0058	0.1105	-9.51	-66.80	-4.70
acetone	1	-77.10	-62.54	-14.56	0.0040	0.1124	-10.18	-72.72	-4.38
acetophenone	1	-64.50	-51.95	-12.55	0.0003	0.0963	-5.25	-57.20	-7.30
water	1	-110.30	-94.33	-15.97	0.0173	0.1436	-25.82	-120.15	9.85
4-methoxyaniline	1	-71.20	-64.58	-6.62	-0.0180	0.0909	-4.43	-69.01	-2.19
4-nitroaniline	1	-75.90	-77.65	1.75	-0.0162	0.0973	-5.81	-83.45	7.55
morpholine	1	-69.60	-63.27	-6.33	-0.0162	0.0860	-3.30	-66.57	-3.03
acetamide	1	-73.90	-67.73	-6.17	-0.0007	0.1070	-8.33	-76.06	2.16
benzamide	1	-67.20	-60.34	-6.86	-0.0008	0.1051	-7.71	-68.05	0.85
dimethyl sulfide	1	-64.50	-58.11	-6.39	0.0160	0.0534	0.89	-57.21	-7.29
dimethyl sulfoxide	1	-67.70	-60.31	-7.39	-0.0045	0.1021	-6.83	-67.14	-0.56
3-chloroaniline	1	-74.70	-68.40	-6.30	-0.0042	0.0941	-4.73	-73.13	-1.57
4-chloroaniline	1	-74.10	-68.70	-5.40	-0.0031	0.0942	-4.75	-73.45	-0.65
PEARSON			0.99					1.00	

Table S 3-2

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/6-31+G* method for the cavity surface with constant density = 0.001 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.25	2.25	0.0003	0.0180	2.83	2.58	-0.58
ethane	0	1.83	-0.24	2.07	-0.0004	0.0158	2.83	2.59	-0.76
n-propane	0	1.96	-0.31	2.27	-0.0006	0.0158	2.83	2.52	-0.56
n-butane	0	2.08	-0.36	2.44	-0.0006	0.0159	2.83	2.47	-0.39
n-pentane	0	2.33	-0.40	2.73	-0.0008	0.0157	2.83	2.42	-0.09
n-hexane	0	2.49	-0.45	2.94	-0.0008	0.0158	2.83	2.37	0.12
n-heptane	0	2.62	-0.50	3.12	-0.0009	0.0152	2.83	2.32	0.30
n-octane	0	2.89	-0.54	3.43	-0.0009	0.0151	2.83	2.29	0.60
2-methylpropane	0	2.32	-0.42	2.74	-0.0006	0.0159	2.83	2.41	-0.09
2,2-dimethylpropane	0	2.50	-0.57	3.07	-0.0006	0.0159	2.83	2.26	0.24
2-methylpentane	0	2.52	-0.49	3.01	-0.0010	0.0157	2.83	2.34	0.18
2,4-dimethylpentane	0	2.88	-0.61	3.49	-0.0011	0.0164	2.83	2.22	0.66
2,2,4-trimethylpentane	0	2.85	-0.73	3.58	-0.0017	0.0171	2.83	2.09	0.76
cyclopropane	0	0.75	-1.14	1.89	-0.0108	0.0210	2.81	1.67	-0.92
cyclopentane	0	1.20	-0.35	1.55	-0.0009	0.0156	2.83	2.48	-1.28
cyclohexane	0	1.23	-0.31	1.54	-0.0009	0.0145	2.83	2.51	-1.28
methylcyclohexane	0	1.71	-0.41	2.12	-0.0009	0.0156	2.83	2.42	-0.71
cis-1,2-dimethylcyclohexane	0	1.58	-0.49	2.07	-0.0010	0.0160	2.83	2.34	-0.76
ethene	0	1.27	-1.51	2.78	-0.0126	0.0255	2.80	1.29	-0.02
propene	0	1.27	-1.43	2.70	-0.0135	0.0238	2.79	1.37	-0.10
1-butene	0	1.38	-1.38	2.76	-0.0138	0.0231	2.79	1.41	-0.03
1-pentene	0	1.66	-1.44	3.10	-0.0138	0.0229	2.79	1.35	0.31
E-2-pentene	0	1.34	-1.23	2.57	-0.0135	0.0216	2.80	1.57	-0.23
1-hexene	0	1.68	-1.56	3.24	-0.0135	0.0232	2.79	1.23	0.45
2-methylpropene	0	1.16	-1.44	2.60	-0.0143	0.0215	2.79	1.35	-0.19
s-trans-1,3-butadiene	0	0.61	-2.55	3.16	-0.0110	0.0262	2.81	0.25	0.36
cyclopentene	0	0.56	-1.16	1.72	-0.0140	0.0246	2.79	1.63	-1.07
ethyne	0	-0.01	-4.29	4.28	-0.0126	0.0550	2.68	-1.61	1.60
propyne	0	-0.31	-3.50	3.19	-0.0149	0.0514	2.69	-0.82	0.51
1-butyne	0	-0.16	-3.40	3.24	-0.0151	0.0514	2.68	-0.72	0.56
1-pentyne	0	0.01	-3.28	3.29	-0.0153	0.0510	2.69	-0.60	0.61
1-hexyne	0	0.29	-3.53	3.82	-0.0153	0.0509	2.69	-0.85	1.14

butenyne	0	0.04	-4.10	4.14	-0.0143	0.0539	2.67	-1.43	1.47
benzene	0	-0.87	-3.31	2.44	-0.0066	0.0277	2.82	-0.49	-0.38
ethylbenzene	0	-0.80	-3.18	2.38	-0.0077	0.0270	2.82	-0.36	-0.44
naphthalene	0	-2.39	-4.74	2.35	-0.0075	0.0282	2.82	-1.92	-0.47
anthracene	0	-4.23	-6.13	1.90	-0.0079	0.0290	2.81	-3.31	-0.92
toluene	0	-0.89	-3.16	2.27	-0.0077	0.0271	2.82	-0.34	-0.55
p-xylene	0	-0.81	-2.98	2.17	-0.0086	0.0253	2.82	-0.16	-0.65
m-xylene	0	-0.84	-3.01	2.17	-0.0088	0.0265	2.82	-0.19	-0.65
o-xylene	0	-0.90	-3.11	2.21	-0.0086	0.0261	2.82	-0.30	-0.60
fluoromethane	0	-0.22	-3.57	3.35	-0.0229	0.0265	2.57	-1.00	0.78
chloromethane	0	-0.56	-3.19	2.63	-0.0118	0.0313	2.80	-0.39	-0.17
bromomethane	0	-0.82	-3.13	2.31	-0.0096	0.0324	2.81	-0.32	-0.50
chlorofluoromethane	0	-0.77	-4.86	4.09	-0.0148	0.0406	2.75	-2.12	1.35
dichloromethane	0	-1.36	-4.35	2.99	-0.0070	0.0428	2.78	-1.57	0.21
dibromomethane	0	-2.11	-4.36	2.25	-0.0053	0.0431	2.78	-1.58	-0.53
chlorodifluoromethane	0	-0.50	-4.44	3.94	-0.0085	0.0514	2.73	-1.71	1.21
chloroform	0	-1.07	-3.69	2.62	-0.0031	0.0519	2.73	-0.96	-0.11
chloroethane	0	-0.63	-3.16	2.53	-0.0126	0.0295	2.80	-0.37	-0.26
bromoethane	0	-0.70	-3.12	2.42	-0.0104	0.0306	2.81	-0.32	-0.38
bromoform	0	-1.98	-4.17	2.19	-0.0023	0.0507	2.73	-1.43	-0.55
tetrafluoromethane	0	3.16	-1.64	4.80	-0.0023	0.0615	2.62	0.98	2.18
difluorodichloromethane	0	1.69	-1.35	3.04	-0.0036	0.0370	2.80	1.45	0.24
fluorotrichloromethane	0	0.82	-1.44	2.26	-0.0042	0.0343	2.81	1.37	-0.55
bromotrifluoromethane	0	1.79	-1.77	3.56	-0.0034	0.0604	2.64	0.87	0.92
bromotrichloromethane	0	-0.93	-1.96	1.03	-0.0007	0.0450	2.77	0.81	-1.74
hexafluoroethane	0	3.94	-1.74	5.68	-0.0025	0.0611	2.63	0.89	3.05
hexachloroethane	0	-1.40	-2.15	0.75	-0.0011	0.0332	2.81	0.66	-2.06
chloropentafluoroethane	0	2.86	-1.60	4.46	-0.0034	0.0573	2.67	1.07	1.79
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.73	3.50	-0.0055	0.0351	2.81	1.07	0.70
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-4.89	5.41	-0.0098	0.0535	2.70	-2.19	2.71
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-4.46	4.33	-0.0059	0.0535	2.71	-1.75	1.62
1-chloro-2,2,2-trifluoroethane	0	0.06	-4.97	5.03	-0.0078	0.0510	2.73	-2.24	2.30
1,1,1,2-tetrachloroethane	0	-1.15	-4.22	3.07	-0.0069	0.0428	2.78	-1.44	0.29
1,1,1-trichloroethane	0	-0.25	-2.82	2.57	-0.0047	0.0317	2.81	-0.01	-0.24
1,1,2-trichloroethane	0	-1.95	-5.27	3.32	-0.0078	0.0455	2.76	-2.51	0.56

1,1-difluoroethane	0	-0.11	-4.64	4.53	-0.0173	0.0352	2.73	-1.91	1.80
1-bromo-2-chloroethane	0	-1.95	-4.55	2.60	-0.0093	0.0356	2.80	-1.75	-0.20
octafluoropropane	0	4.28	-2.00	6.28	-0.0024	0.0595	2.65	0.65	3.63
2-chloropropane	0	-0.25	-3.13	2.88	-0.0133	0.0282	2.79	-0.34	0.09
1-chloropropane	0	-0.27	-3.12	2.85	-0.0126	0.0288	2.80	-0.33	0.06
1-bromopropane	0	-0.56	-3.11	2.55	-0.0105	0.0300	2.81	-0.31	-0.25
2-bromopropane	0	-0.48	-3.10	2.62	-0.0112	0.0295	2.80	-0.29	-0.19
2-chlorobutane	0	0.07	-2.97	3.04	-0.0135	0.0278	2.79	-0.18	0.25
1-bromobutane	0	-0.41	-3.17	2.76	-0.0106	0.0300	2.81	-0.36	-0.05
1-chloropentane	0	0.07	-3.23	3.30	-0.0128	0.0286	2.80	-0.43	0.50
2-chloropentane	0	0.07	-2.98	3.05	-0.0135	0.0274	2.79	-0.19	0.26
1-bromopentane	0	-0.08	-3.21	3.13	-0.0106	0.0300	2.81	-0.40	0.32
1-bromo-isobutane	0	-0.03	-2.99	2.96	-0.0106	0.0302	2.81	-0.18	0.15
tetrachloroethene	0	0.05	-1.81	1.86	-0.0018	0.0324	2.81	1.01	-0.96
trichloroethene	0	-0.39	-2.79	2.40	-0.0034	0.0485	2.75	-0.04	-0.35
chloroethene	0	-0.59	-2.82	2.23	-0.0091	0.0380	2.79	-0.03	-0.56
E-1,2-dichloroethene	0	-0.76	-3.12	2.36	-0.0060	0.0438	2.78	-0.35	-0.41
Z-1,2-dichloroethene	0	-1.17	-3.93	2.76	-0.0059	0.0446	2.77	-1.16	-0.01
3-chloropropene	0	-0.57	-3.73	3.16	-0.0114	0.0317	2.80	-0.93	0.36
3-bromopropene	0	-0.86	-4.18	3.32	-0.0102	0.0334	2.80	-1.38	0.52
fluorobenzene	0	-0.78	-3.95	3.17	-0.0175	0.0329	2.73	-1.22	0.44
chlorobenzene	0	-1.12	-3.70	2.58	-0.0085	0.0329	2.81	-0.89	-0.23
bromobenzene	0	-1.46	-3.79	2.33	-0.0070	0.0331	2.81	-0.98	-0.48
1,4-dichlorobenzene	0	-1.01	-3.87	2.86	-0.0070	0.0368	2.80	-1.07	0.06
1,2-dichlorobenzene	0	-1.36	-4.07	2.71	-0.0075	0.0363	2.80	-1.27	-0.09
p-dibromobenzene	0	-2.30	-4.05	1.75	-0.0056	0.0365	2.80	-1.25	-1.05
chlorotoluene	0	-1.92	-5.89	3.97	-0.0128	0.0324	2.79	-3.10	1.18
o-chlorotoluene	0	-1.15	-3.38	2.23	-0.0091	0.0327	2.81	-0.57	-0.58
bromotoluene	0	-2.37	-5.89	3.52	-0.0107	0.0338	2.80	-3.09	0.72
p-bromotoluene	0	-1.39	-3.70	2.31	-0.0074	0.0327	2.81	-0.89	-0.50
2,3-dichlorobiphenyl	0	-2.45	-5.86	3.41	-0.0080	0.0356	2.80	-3.05	0.60
2,2'-dichlorobiphenyl	0	-2.73	-6.34	3.61	-0.0093	0.0330	2.81	-3.53	0.80
2,2',3'-trichlorobiphenyl	0	-1.99	-6.22	4.23	-0.0098	0.0361	2.80	-3.42	1.43
1,2-dimethoxyethane	0	-4.84	-5.08	0.24	-0.0319	0.0213	1.86	-3.22	-1.62
anisole	0	-2.45	-5.15	2.70	-0.0285	0.0295	2.21	-2.94	0.49

dimethyl ether	0	-1.92	-3.48	1.56	-0.0332	0.0213	1.68	-1.80	-0.12
diethyl ether	0	-1.76	-3.46	1.70	-0.0342	0.0195	1.55	-1.91	0.15
isopropyl ether	0	-0.53	-3.25	2.72	-0.0342	0.0196	1.53	-1.71	1.18
methyl propyl ether	0	-1.66	-3.24	1.58	-0.0330	0.0205	1.71	-1.53	-0.13
methyl isopropyl ether	0	-2.01	-3.23	1.22	-0.0333	0.0201	1.67	-1.56	-0.45
t-butyl methyl ether	0	-2.21	-3.20	0.99	-0.0334	0.0196	1.65	-1.54	-0.67
ethyl phenyl ether	0	-2.22	-4.96	2.74	-0.0286	0.0293	2.20	-2.76	0.54
tetrahydrofuran	0	-3.47	-3.88	0.41	-0.0350	0.0208	1.42	-2.46	-1.01
tetrahydropyran	0	-3.12	-3.49	0.37	-0.0345	0.0194	1.50	-1.99	-1.13
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-6.02	5.90	-0.0212	0.0490	2.57	-3.46	3.34
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-7.31	7.42	-0.0140	0.0538	2.67	-4.63	4.74
acetaldehyde	0	-3.50	-6.87	3.37	-0.0331	0.0353	1.69	-5.18	1.68
propanal	0	-3.44	-6.43	2.99	-0.0332	0.0341	1.67	-4.76	1.32
butanal	0	-3.18	-6.61	3.43	-0.0331	0.0334	1.69	-4.92	1.74
pentanal	0	-3.03	-6.50	3.47	-0.0334	0.0335	1.64	-4.86	1.83
octanal	0	-2.29	-6.67	4.38	-0.0331	0.0336	1.68	-4.99	2.70
benzaldehyde	0	-4.02	-7.96	3.94	-0.0337	0.0348	1.60	-6.37	2.35
p-hydroxybenzaldehyde	0	-10.48	-13.80	3.32	-0.0348	0.0945	0.26	-13.54	3.06
m-hydroxybenzaldehyde	0	-9.51	-13.23	3.72	-0.0332	0.0938	0.53	-12.69	3.18
acetone	0	-3.85	-6.98	3.13	-0.0344	0.0332	1.49	-5.50	1.65
2-butanone	0	-3.64	-6.52	2.88	-0.0347	0.0322	1.44	-5.08	1.44
2-pentanone	0	-3.53	-6.53	3.00	-0.0347	0.0320	1.45	-5.08	1.55
3-pentanone	0	-3.41	-6.06	2.65	-0.0338	0.0317	1.59	-4.47	1.06
2-hexanone	0	-3.29	-6.60	3.31	-0.0347	0.0319	1.45	-5.15	1.86
2-heptanone	0	-3.04	-6.64	3.60	-0.0348	0.0309	1.43	-5.21	2.17
4-heptanone	0	-2.93	-6.09	3.16	-0.0339	0.0316	1.58	-4.51	1.58
2-octanone	0	-2.88	-6.69	3.81	-0.0346	0.0292	1.47	-5.22	2.34
5-nonanone	0	-2.67	-6.19	3.52	-0.0340	0.0311	1.56	-4.63	1.96
3,3-dimethylbutanone	0	-2.89	-6.18	3.29	-0.0349	0.0288	1.42	-4.76	1.87
cyclopentanone	0	-4.68	-6.98	2.30	-0.0347	0.0320	1.45	-5.54	0.86
acetophenone	0	-4.58	-7.86	3.28	-0.0350	0.0327	1.40	-6.46	1.88
methyl formate	0	-2.78	-6.89	4.11	-0.0308	0.0406	1.96	-4.93	2.15
ethyl formate	0	-2.65	-6.77	4.12	-0.0312	0.0400	1.91	-4.86	2.21
methyl acetate	0	-3.32	-6.47	3.15	-0.0325	0.0381	1.75	-4.73	1.41
ethyl acetate	0	-3.10	-6.40	3.30	-0.0328	0.0371	1.71	-4.69	1.59

propyl acetate	0	-2.86	-6.42	3.56	-0.0329	0.0363	1.70	-4.71	1.85
butyl acetate	0	-2.55	-6.52	3.97	-0.0328	0.0368	1.71	-4.80	2.25
methyl propanoate	0	-2.93	-6.15	3.22	-0.0321	0.0373	1.81	-4.35	1.42
methyl butanoate	0	-2.83	-6.18	3.35	-0.0321	0.0372	1.81	-4.38	1.55
methyl pentanoate	0	-2.57	-6.25	3.68	-0.0323	0.0369	1.79	-4.46	1.89
methyl hexanoate	0	-2.49	-6.30	3.81	-0.0321	0.0367	1.81	-4.49	2.00
methyl benzoate	0	-3.91	-7.03	3.12	-0.0323	0.0354	1.78	-5.25	1.34
hydrogen	0	2.33	-0.11	2.44	0.0014	0.0163	2.83	2.71	-0.38
water	0	-6.31	-9.80	3.49	-0.0337	0.0816	0.95	-8.85	2.54
water dimer	0	-11.27	-15.27	4.00	-0.0377	0.0892	-0.04	-15.31	4.04
hydrogen peroxide	0	-8.58	-10.99	2.41	-0.0272	0.0923	1.24	-9.75	1.17
methyl peroxide	0	-5.28	-8.08	2.80	-0.0281	0.0915	1.21	-6.87	1.59
ethyl peroxide	0	-5.32	-8.02	2.70	-0.0285	0.0903	1.23	-6.79	1.47
1,4-dioxane	0	-5.05	-6.09	1.04	-0.0325	0.0244	1.78	-4.31	-0.74
methanol	0	-5.11	-6.65	1.54	-0.0337	0.0783	1.06	-5.59	0.48
ethanol	0	-5.01	-6.29	1.28	-0.0336	0.0783	1.08	-5.21	0.20
1-propanol	0	-4.83	-6.28	1.45	-0.0336	0.0772	1.11	-5.17	0.34
isopropanol	0	-4.76	-6.13	1.37	-0.0343	0.0736	1.09	-5.04	0.28
1-butanol	0	-4.72	-6.34	1.62	-0.0337	0.0768	1.11	-5.23	0.51
t-butanol	0	-4.51	-5.89	1.38	-0.0339	0.0736	1.15	-4.74	0.23
1-pentanol	0	-4.47	-6.51	2.04	-0.0342	0.0749	1.07	-5.43	0.96
1-hexanol	0	-4.36	-6.61	2.25	-0.0343	0.0759	1.04	-5.57	1.21
1-heptanol	0	-4.24	-6.78	2.54	-0.0343	0.0744	1.07	-5.70	1.46
1-octanol	0	-4.09	-5.78	1.69	-0.0340	0.0704	1.21	-4.57	0.48
allyl alcohol	0	-5.08	-6.67	1.59	-0.0336	0.0774	1.11	-5.56	0.48
cyclopentanol	0	-5.49	-5.80	0.31	-0.0344	0.0707	1.15	-4.65	-0.84
2-methoxyethanol	0	-6.77	-8.82	2.05	-0.0328	0.0802	1.13	-7.69	0.92
2,2,2-trifluoroethanol	0	-4.31	-10.32	6.01	-0.0262	0.0922	1.31	-9.01	4.70
1,1,1-trifluoropropan-2-ol	0	-4.16	-7.29	3.13	-0.0288	0.0856	1.40	-5.89	1.73
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-8.47	4.70	-0.0227	0.0982	1.19	-7.28	3.51
phenol	0	-6.62	-8.62	2.00	-0.0277	0.0895	1.33	-7.30	0.68
p-bromophenol	0	-7.13	-9.32	2.19	-0.0259	0.0909	1.40	-7.92	0.79
o-cresol	0	-5.87	-7.98	2.11	-0.0272	0.0888	1.40	-6.58	0.71
m-cresol	0	-5.49	-8.43	2.94	-0.0280	0.0898	1.29	-7.15	1.66
p-cresol	0	-6.14	-8.39	2.25	-0.0282	0.0890	1.31	-7.09	0.95

1,2-ethanediol	0	-9.30	-10.80	1.50	-0.0353	0.0850	0.60	-10.20	0.90
acetic acid	0	-6.70	-9.53	2.83	-0.0317	0.0987	0.45	-9.08	2.38
propanoic acid	0	-6.47	-9.19	2.72	-0.0312	0.0986	0.53	-8.67	2.20
butanoic acid	0	-6.36	-9.21	2.85	-0.0312	0.0982	0.54	-8.66	2.30
pentanoic acid	0	-6.16	-9.27	3.11	-0.0310	0.0980	0.58	-8.69	2.53
hexanoic acid	0	-6.21	-9.31	3.10	-0.0313	0.0984	0.53	-8.78	2.57
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-15.85	3.89	-0.0276	0.1030	0.59	-15.26	3.30
ammonia	0	-4.29	-6.03	1.74	-0.0383	0.0459	0.73	-5.30	1.01
methylamine	0	-4.56	-4.63	0.07	-0.0376	0.0439	0.88	-3.75	-0.81
ethylamine	0	-4.50	-4.73	0.23	-0.0377	0.0428	0.87	-3.86	-0.64
butylamine	0	-4.29	-4.79	0.50	-0.0377	0.0427	0.87	-3.93	-0.36
propylamine	0	-4.39	-4.76	0.37	-0.0377	0.0432	0.86	-3.90	-0.49
pentylamine	0	-4.10	-4.82	0.72	-0.0379	0.0421	0.83	-3.99	-0.11
dimethylamine	0	-4.29	-3.37	-0.92	-0.0361	0.0435	1.16	-2.20	-2.09
diethylamine	0	-4.07	-3.26	-0.81	-0.0359	0.0416	1.21	-2.05	-2.02
dipropylamine	0	-3.66	-3.32	-0.34	-0.0356	0.0416	1.26	-2.06	-1.60
trimethylamine	0	-3.23	-2.17	-1.06	-0.0344	0.0185	1.50	-0.66	-2.57
azetidine	0	-5.56	-3.79	-1.77	-0.0376	0.0431	0.88	-2.91	-2.65
pyrrolidine	0	-5.48	-4.01	-1.47	-0.0375	0.0421	0.90	-3.11	-2.37
piperidine	0	-5.11	-2.94	-2.17	-0.0356	0.0433	1.26	-1.68	-3.43
2-methoxyethanamine	0	-6.55	-7.61	1.06	-0.0366	0.0451	1.06	-6.55	0.00
1,2-ethanediamine	0	-9.72	-9.17	-0.55	-0.0367	0.0452	1.04	-8.13	-1.59
nitromethane	0	-3.95	-9.06	5.11	-0.0252	0.0421	2.42	-6.64	2.69
nitroethane	0	-3.71	-8.49	4.78	-0.0259	0.0389	2.39	-6.11	2.40
1-nitropropane	0	-3.34	-8.34	5.00	-0.0258	0.0385	2.39	-5.95	2.61
2-nitropropane	0	-3.14	-7.69	4.55	-0.0263	0.0373	2.36	-5.32	2.18
1-nitrobutane	0	-3.08	-8.36	5.28	-0.0260	0.0383	2.38	-5.98	2.90
nitrobenzene	0	-4.12	-7.77	3.65	-0.0251	0.0399	2.43	-5.34	1.22
2-methyl-1-nitrobenzene	0	-3.59	-7.31	3.72	-0.0262	0.0380	2.37	-4.95	1.36
pyridine	0	-4.70	-5.41	0.71	-0.0354	0.0347	1.32	-4.09	-0.61
2-methylpyridine	0	-4.63	-4.95	0.32	-0.0355	0.0333	1.31	-3.63	-1.00
3-methylpyridine	0	-4.77	-5.31	0.54	-0.0358	0.0328	1.25	-4.06	-0.71
4-methylpyridine	0	-4.94	-5.46	0.52	-0.0363	0.0304	1.18	-4.28	-0.66
4-ethylpyridine	0	-4.74	-5.42	0.68	-0.0362	0.0305	1.19	-4.24	-0.50
2,4-dimethylpyridine	0	-4.86	-5.00	0.14	-0.0363	0.0290	1.18	-3.82	-1.04

2,5-dimethylpyridine	0	-4.72	-4.85	0.13	-0.0357	0.0319	1.27	-3.57	-1.15
2,6-dimethylpyridine	0	-4.60	-4.53	-0.07	-0.0355	0.0329	1.31	-3.21	-1.39
3,4-dimethylpyridine	0	-5.22	-5.47	0.25	-0.0365	0.0301	1.13	-4.34	-0.88
3,5-dimethylpyridine	0	-4.84	-5.23	0.39	-0.0362	0.0316	1.19	-4.04	-0.80
aniline	0	-5.49	-7.66	2.17	-0.0301	0.0568	1.91	-5.75	0.26
N-methylaniline	0	-4.68	-6.08	1.40	-0.0269	0.0563	2.20	-3.88	-0.80
2-methylaniline	0	-5.56	-7.02	1.46	-0.0305	0.0550	1.89	-5.13	-0.43
3-methylaniline	0	-5.67	-7.46	1.79	-0.0304	0.0559	1.90	-5.56	-0.11
4-methylaniline	0	-5.55	-7.40	1.85	-0.0307	0.0543	1.88	-5.52	-0.03
N-ethylaniline	0	-4.62	-5.91	1.29	-0.0244	0.0577	2.34	-3.56	-1.06
3-aminoaniline	0	-9.92	-11.99	2.07	-0.0302	0.0562	1.92	-10.08	0.16
N,N-dimethylaniline	0	-3.58	-4.56	0.98	-0.0225	0.0262	2.59	-1.97	-1.61
piperazine	0	-7.40	-5.48	-1.92	-0.0354	0.0441	1.29	-4.19	-3.21
N-methylpiperazine	0	-7.77	-4.41	-3.36	-0.0353	0.0445	1.31	-3.10	-4.67
N,N'-dimethylpiperazine	0	-7.58	-3.29	-4.29	-0.0335	0.0188	1.65	-1.64	-5.94
1-methylthymine	0	-10.40	-15.36	4.96	-0.0352	0.0836	0.66	-14.70	4.30
9-methyladenine	0	-13.60	-13.01	-0.59	-0.0357	0.0703	0.95	-12.06	-1.54
acetamide	0	-9.71	-11.75	2.04	-0.0374	0.0705	0.62	-11.13	1.42
E-N-methylacetamide	0	-10.00	-10.38	0.38	-0.0387	0.0649	0.43	-9.95	-0.05
Z-N-methylacetamide	0	-10.00	-9.85	-0.15	-0.0390	0.0706	0.26	-9.59	-0.41
benzamide	0	-10.90	-12.11	1.21	-0.0367	0.0698	0.77	-11.34	0.44
2,6-dichlorothiobenzamide	0	-10.81	-14.39	3.58	-0.0232	0.0851	1.79	-12.60	1.79
urea	0	-13.80	-14.67	0.87	-0.0365	0.0687	0.83	-13.84	0.04
1,1-dimethyl-3-phenylurea	0	-9.63	-11.31	1.68	-0.0352	0.0690	1.05	-10.26	0.63
hydrazine	0	-6.26	-7.87	1.61	-0.0350	0.0468	1.34	-6.53	0.27
methylhydrazine	0	-5.31	-7.18	1.87	-0.0353	0.0471	1.30	-5.88	0.57
1,1-dimethylhydrazine	0	-4.48	-5.78	1.30	-0.0354	0.0474	1.28	-4.50	0.02
2-methylpyrazine	0	-5.57	-5.52	-0.05	-0.0313	0.0338	1.91	-3.60	-1.97
2-ethylpyrazine	0	-5.51	-5.16	-0.35	-0.0314	0.0336	1.90	-3.25	-2.26
morpholine	0	-7.17	-5.91	-1.26	-0.0340	0.0466	1.50	-4.41	-2.76
N-methylmorpholine	0	-6.34	-4.71	-1.63	-0.0337	0.0216	1.61	-3.10	-3.24
acetonitrile	0	-3.89	-7.48	3.59	-0.0298	0.0369	2.07	-5.41	1.52
butanonitrile	0	-3.64	-6.86	3.22	-0.0299	0.0342	2.07	-4.79	1.15
propionitrile	0	-3.85	-7.09	3.24	-0.0299	0.0341	2.06	-5.03	1.18
benzonitrile	0	-4.10	-7.82	3.72	-0.0292	0.0384	2.12	-5.69	1.59

2,6-dichlorobenzonitrile	0	-5.22	-8.18	2.96	-0.0278	0.0421	2.23	-5.95	0.73
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-10.98	1.98	-0.0276	0.0827	1.60	-9.38	0.38
trimethylphosphate	0	-8.70	-11.10	2.40	-0.0364	0.0489	1.09	-10.01	1.31
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-10.59	3.98	-0.0323	0.0559	1.67	-8.93	2.32
phosphine	0	0.60	-0.98	1.58	-0.0133	0.0265	2.79	1.81	-1.21
hydrogen sulfide	0	-0.70	-2.97	2.27	-0.0150	0.0318	2.77	-0.20	-0.50
dimethyl sulfide	0	-1.54	-3.11	1.57	-0.0194	0.0256	2.69	-0.42	-1.12
diethyl sulfide	0	-1.43	-2.91	1.48	-0.0202	0.0213	2.67	-0.24	-1.19
dipropyl sulfide	0	-1.27	-3.02	1.75	-0.0204	0.0209	2.67	-0.35	-0.92
bis(2-chloroethyl)sulfide	0	-3.92	-6.90	2.98	-0.0148	0.0327	2.77	-4.13	0.21
dimethyl disulfide	0	-1.83	-3.93	2.10	-0.0157	0.0287	2.77	-1.16	-0.67
diethyl disulfide	0	-1.63	-3.50	1.87	-0.0164	0.0262	2.76	-0.74	-0.89
methanethiol	0	-1.24	-3.06	1.82	-0.0177	0.0271	2.73	-0.32	-0.92
ethanethiol	0	-1.30	-3.00	1.70	-0.0179	0.0262	2.73	-0.26	-1.04
1-propanethiol	0	-1.05	-3.04	1.99	-0.0179	0.0261	2.73	-0.31	-0.74
thiophene	0	-1.42	-3.77	2.35	-0.0090	0.0372	2.80	-0.98	-0.44
thiophenol	0	-2.55	-5.11	2.56	-0.0143	0.0323	2.78	-2.34	-0.21
thioanisole	0	-2.73	-5.16	2.43	-0.0164	0.0295	2.75	-2.41	-0.32
tetramethylsilane	0	3.04	-1.22	4.26	-0.0048	0.0192	2.83	1.60	1.44
acetylene	-1	-76.50	-67.18	-9.32	-0.0567	0.0192	-7.38	-74.55	-1.95
acetonitrile	-1	-66.60	-61.21	-5.39	-0.0535	0.0023	-5.26	-66.47	-0.13
cyanamide	-1	-72.20	-65.91	-6.29	-0.0544	0.0244	-5.83	-71.74	-0.46
aniline	-1	-62.90	-57.63	-5.27	-0.0597	0.0133	-9.79	-67.42	4.52
diphenylamine	-1	-54.60	-50.77	-3.83	-0.0532	0.0163	-5.08	-55.85	1.25
hydrogen cyanide	-1	-70.20	-67.21	-2.99	-0.0539	-0.0345	-5.48	-72.69	2.49
formic acid	-1	-76.20	-68.17	-8.03	-0.0569	0.0026	-7.52	-75.69	-0.51
acetic acid	-1	-77.60	-67.74	-9.86	-0.0582	0.0085	-8.53	-76.27	-1.33
propanoic acid	-1	-76.20	-65.80	-10.40	-0.0582	0.0078	-8.57	-74.37	-1.83
hexanoic acid	-1	-74.60	-65.08	-9.52	-0.0582	0.0148	-8.58	-73.66	-0.94
acrylic acid	-1	-74.00	-66.42	-7.58	-0.0579	0.0191	-8.30	-74.72	0.72
pyruvic acid	-1	-68.50	-65.63	-2.87	-0.0548	0.0263	-6.07	-71.69	3.19
benzoic acid	-1	-71.20	-63.91	-7.29	-0.0571	0.0230	-7.72	-71.63	0.43
methanol	-1	-95.00	-70.98	-24.02	-0.0687	-0.0160	-19.63	-90.60	-4.40
ethanol	-1	-90.70	-68.04	-22.66	-0.0691	0.0013	-20.16	-88.20	-2.50
1-propanol	-1	-88.30	-67.25	-21.05	-0.0691	0.0074	-20.23	-87.48	-0.82

isopropanol	-1	-86.30	-65.33	-20.97	-0.0686	0.0014	-19.56	-84.90	-1.40
2-butanol	-1	-84.20	-62.10	-22.10	-0.0682	0.0016	-18.98	-81.08	-3.12
t-butanol	-1	-82.30	-62.97	-19.33	-0.0680	0.0019	-18.66	-81.63	-0.67
allyl alcohol	-1	-86.60	-66.93	-19.67	-0.0688	0.0111	-19.78	-86.71	0.11
benzyl alcohol	-1	-85.10	-62.87	-22.23	-0.0674	0.0190	-17.97	-80.84	-4.26
2-methoxyethanol	-1	-89.40	-68.84	-20.56	-0.0688	0.0134	-19.77	-88.62	-0.78
phenol	-1	-71.90	-59.91	-11.99	-0.0606	0.0141	-10.60	-70.52	-1.38
2-methylphenol	-1	-70.20	-58.00	-12.20	-0.0607	0.0127	-10.71	-68.71	-1.49
3-methylphenol	-1	-71.10	-59.80	-11.30	-0.0608	0.0135	-10.78	-70.59	-0.51
4-methylphenol	-1	-72.00	-59.85	-12.15	-0.0613	0.0130	-11.25	-71.09	-0.91
1,2-ethanediol	-1	-85.30	-72.27	-13.03	-0.0689	0.0668	-20.17	-92.44	7.14
3-hydroxyphenol	-1	-73.80	-62.38	-11.42	-0.0595	0.0775	-10.18	-72.55	-1.25
4-hydroxyphenol	-1	-77.60	-64.42	-13.18	-0.0614	0.0734	-11.73	-76.15	-1.45
methyl hydroperoxide	-1	-93.20	-73.31	-19.89	-0.0670	0.0025	-17.41	-90.72	-2.48
ethyl hydroperoxide	-1	-89.20	-72.35	-16.86	-0.0671	0.0110	-17.53	-89.88	0.68
acetaldehyde	-1	-76.50	-64.42	-12.08	-0.0618	0.0008	-11.71	-76.13	-0.37
acetone	-1	-76.20	-63.32	-12.88	-0.0622	0.0060	-12.13	-75.45	-0.75
3-pentanone	-1	-73.70	-58.25	-15.45	-0.0612	0.0077	-11.17	-69.43	-4.27
water	-1	-104.70	-81.77	-22.93	-0.0729	0.0047	-25.76	-107.53	2.83
hydrogen peroxide	-1	-97.30	-78.74	-18.56	-0.0669	0.0440	-17.34	-96.08	-1.22
hydroperoxyl radical	-1	-83.30	-74.02	-9.28	-0.0585	-0.0463	-8.80	-82.82	-0.48
2-nitrophenol	-1	-60.10	-57.82	-2.28	-0.0541	0.0243	-5.63	-63.44	3.34
3-nitrophenol	-1	-61.90	-54.45	-7.45	-0.0570	0.0299	-7.60	-62.05	0.15
4-nitrophenol	-1	-57.80	-52.52	-5.28	-0.0524	0.0265	-4.58	-57.10	-0.70
nitromethane	-1	-76.50	-65.87	-10.63	-0.0557	0.0148	-6.65	-72.52	-3.98
4-nitroaniline	-1	-57.40	-52.06	-5.34	-0.0509	0.0252	-3.74	-55.80	-1.60
acetamide	-1	-80.20	-64.86	-15.34	-0.0586	0.0086	-8.88	-73.74	-6.46
methanethiol	-1	-73.80	-63.18	-10.62	-0.0458	0.0018	-1.45	-64.63	-9.17
ethanethiol	-1	-71.80	-61.29	-10.51	-0.0458	0.0063	-1.43	-62.72	-9.08
1-propanethiol	-1	-70.50	-60.97	-9.53	-0.0458	0.0105	-1.45	-62.42	-8.08
thiophenol	-1	-63.40	-57.23	-6.17	-0.0418	0.0188	-0.12	-57.35	-6.05
hydrogen sulfide	-1	-72.10	-64.45	-7.65	-0.0450	-0.0076	-1.13	-65.58	-6.52
dimethyl sulfoxide	-1	-67.70	-62.03	-5.67	-0.0595	0.0150	-9.62	-71.65	3.95
hydrofluoric acid	-1	-104.40	-87.24	-17.16	-0.0759	-0.0759	-30.97	-118.20	13.80
hydrochloric acid	-1	-74.50	-68.54	-5.96	-0.0449	-0.0449	-1.11	-69.64	-4.86

hydrobromic acid	-1	-68.30	-64.22	-4.08	-0.0387	-0.0387	0.69	-63.53	-4.77
chloroform	-1	-54.10	-51.34	-2.76	-0.0415	-0.0047	-0.02	-51.36	-2.74
trifluoroacetic acid	-1	-59.30	-59.75	0.45	-0.0512	0.0421	-3.96	-63.71	4.41
chloroacetic acid	-1	-69.70	-62.79	-6.91	-0.0544	0.0204	-5.78	-68.58	-1.12
dichloroacetic acid	-1	-62.30	-58.85	-3.45	-0.0516	0.0283	-4.13	-62.98	0.68
2,2,2-trifluoroethanol	-1	-77.50	-63.17	-14.33	-0.0648	0.0187	-14.86	-78.02	0.52
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-57.89	-7.61	-0.0605	0.0278	-10.49	-68.38	2.88
2-chlorophenol	-1	-66.10	-57.45	-8.65	-0.0583	0.0203	-8.64	-66.09	-0.01
4-chlorophenol	-1	-66.00	-55.71	-10.29	-0.0588	0.0202	-9.07	-64.79	-1.21
methylamine	1	-76.40	-75.92	-0.48	0.0262	0.1099	0.61	-75.31	-1.09
n-propylamine	1	-71.50	-71.22	-0.28	0.0063	0.1093	0.66	-70.55	-0.95
isopropylamine	1	-69.60	-69.56	-0.04	0.0093	0.1074	0.81	-68.75	-0.85
tert-butylamine	1	-67.30	-66.98	-0.32	0.0092	0.1061	0.91	-66.08	-1.22
cyclohexanamine	1	-68.70	-66.66	-2.04	0.0068	0.1064	0.89	-65.77	-2.93
allylamine	1	-72.00	-71.42	-0.58	-0.0091	0.1106	0.54	-70.88	-1.12
dimethylamine	1	-68.60	-68.07	-0.53	0.0240	0.1049	0.99	-67.07	-1.53
diethylamine	1	-63.40	-62.30	-1.10	0.0098	0.1000	1.32	-60.98	-2.42
di-n-propylamine	1	-60.50	-60.23	-0.27	0.0067	0.0998	1.34	-58.90	-1.60
diallylamine	1	-61.60	-61.03	-0.57	-0.0074	0.1021	1.19	-59.85	-1.75
trimethylamine	1	-61.10	-61.29	0.19	0.0231	0.1010	1.26	-60.03	-1.07
triethylamine	1	-54.60	-53.91	-0.69	0.0079	0.0904	1.83	-52.08	-2.52
aniline	1	-72.40	-71.86	-0.54	0.0012	0.1146	0.19	-71.67	-0.73
2-methylaniline	1	-70.30	-69.57	-0.73	0.0003	0.1132	0.32	-69.24	-1.06
3-methylaniline	1	-69.60	-70.24	0.64	-0.0002	0.1143	0.22	-70.02	0.42
4-methylaniline	1	-69.80	-70.06	0.26	0.0004	0.1137	0.28	-69.78	-0.02
3-aminoaniline	1	-65.80	-73.29	7.49	-0.0192	0.1139	0.14	-73.15	7.35
N-methylaniline	1	-62.60	-64.02	1.42	0.0008	0.1076	0.79	-63.23	0.63
N-ethylaniline	1	-62.20	-61.30	-0.90	0.0004	0.1053	0.96	-60.34	-1.86
N,N-dimethylaniline	1	-57.20	-57.23	0.03	0.0006	0.1014	1.23	-56.00	-1.20
4-methyl-N,N-dimethylaniline	1	-55.90	-55.76	-0.14	0.0002	0.1004	1.29	-54.46	-1.44
N,N-diethylaniline	1	-54.00	-52.96	-1.04	-0.0001	0.0952	1.60	-51.36	-2.64
1-aminonaphthalene	1	-67.40	-69.03	1.63	-0.0016	0.1157	0.08	-68.95	1.55
aziridine	1	-70.90	-69.58	-1.32	0.0254	0.1108	0.54	-69.04	-1.86
azetidine	1	-67.70	-65.68	-2.02	0.0167	0.1044	1.03	-64.65	-3.05
pyrrolidine	1	-66.00	-63.77	-2.23	0.0112	0.1038	1.07	-62.69	-3.31

piperidine	1	-64.20	-62.12	-2.08	0.0118	0.1045	1.02	-61.10	-3.10
azacycloheptane	1	-63.30	-60.61	-2.69	0.0063	0.1046	1.02	-59.60	-3.70
pyrrole	1	-61.40	-62.28	0.88	0.0107	0.1115	0.48	-61.80	0.40
pyridine	1	-61.10	-61.03	-0.07	0.0142	0.1157	0.09	-60.94	-0.16
quinoline	1	-56.00	-55.83	-0.17	0.0033	0.1090	0.68	-55.15	-0.85
piperazine	1	-66.00	-64.84	-1.16	-0.0243	0.1050	0.67	-64.16	-1.84
acetonitrile	1	-75.30	-70.78	-4.52	0.0307	0.1546	-6.15	-76.93	1.63
ammonia	1	-85.20	-85.81	0.61	0.0552	0.1163	0.03	-85.78	0.58
hydrazine	1	-84.60	-84.70	0.10	-0.0120	0.1148	0.15	-84.55	-0.05
methanol	1	-93.00	-83.84	-9.16	0.0113	0.1615	-7.93	-91.77	-1.23
ethanol	1	-88.40	-78.59	-9.81	0.0055	0.1599	-7.49	-86.08	-2.32
dimethyl ether	1	-79.70	-70.23	-9.47	0.0079	0.1531	-5.81	-76.04	-3.66
diethyl ether	1	-71.50	-62.60	-8.90	0.0039	0.1414	-3.40	-66.00	-5.50
acetone	1	-77.10	-68.54	-8.56	0.0022	0.1428	-3.67	-72.20	-4.90
acetophenone	1	-64.50	-57.54	-6.96	-0.0015	0.1237	-0.77	-58.31	-6.19
water	1	-110.30	-102.38	-7.92	0.0165	0.1752	-12.19	-114.57	4.27
4-methoxyaniline	1	-71.20	-71.45	0.25	-0.0227	0.1132	0.08	-71.37	0.17
4-nitroaniline	1	-75.90	-85.78	9.88	-0.0193	0.1195	-0.42	-86.20	10.30
morpholine	1	-69.60	-69.30	-0.30	-0.0208	0.1081	0.59	-68.72	-0.88
acetamide	1	-73.90	-74.38	0.48	-0.0031	0.1359	-2.47	-76.85	2.95
benzamide	1	-67.20	-67.13	-0.07	-0.0035	0.1336	-2.12	-69.24	2.04
dimethyl sulfide	1	-64.50	-63.06	-1.44	0.0179	0.0694	2.49	-60.57	-3.93
dimethyl sulfoxide	1	-67.70	-66.38	-1.32	-0.0077	0.1298	-1.57	-67.94	0.24
3-chloroaniline	1	-74.70	-75.22	0.52	-0.0057	0.1158	0.08	-75.14	0.44
4-chloroaniline	1	-74.10	-75.54	1.44	-0.0038	0.1171	-0.05	-75.60	1.50
PEARSON			0.99					1.00	

Table S 3-3

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/6-31+G* method for the cavity surface with constant density = 0.002 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.47	2.47	0.0038	0.0318	5.24	4.77	-2.77
ethane	0	1.83	-0.47	2.30	0.0029	0.0285	5.24	4.77	-2.94
n-propane	0	1.96	-0.58	2.54	0.0027	0.0285	5.24	4.66	-2.70
n-butane	0	2.08	-0.68	2.76	0.0027	0.0286	5.24	4.56	-2.48
n-pentane	0	2.33	-0.77	3.10	0.0025	0.0284	5.24	4.47	-2.14
n-hexane	0	2.49	-0.85	3.34	0.0025	0.0285	5.24	4.39	-1.90
n-heptane	0	2.62	-0.93	3.55	0.0023	0.0277	5.24	4.30	-1.68
n-octane	0	2.89	-1.01	3.90	0.0023	0.0276	5.24	4.23	-1.34
2-methylpropane	0	2.32	-0.78	3.10	0.0026	0.0286	5.24	4.46	-2.14
2,2-dimethylpropane	0	2.50	-1.03	3.53	0.0026	0.0287	5.24	4.21	-1.71
2-methylpentane	0	2.52	-0.93	3.45	0.0020	0.0285	5.24	4.31	-1.79
2,4-dimethylpentane	0	2.88	-1.13	4.01	0.0020	0.0293	5.24	4.11	-1.23
2,2,4-trimethylpentane	0	2.85	-1.35	4.20	0.0010	0.0295	5.24	3.89	-1.04
cyclopropane	0	0.75	-1.88	2.63	-0.0105	0.0358	5.23	3.36	-2.61
cyclopentane	0	1.20	-0.66	1.86	0.0023	0.0282	5.24	4.58	-3.38
cyclohexane	0	1.23	-0.62	1.85	0.0024	0.0267	5.24	4.61	-3.38
methylcyclohexane	0	1.71	-0.79	2.50	0.0023	0.0282	5.24	4.45	-2.74
cis-1,2-dimethylcyclohexane	0	1.58	-0.94	2.52	0.0012	0.0287	5.24	4.30	-2.72
ethene	0	1.27	-2.28	3.55	-0.0125	0.0418	5.23	2.95	-1.68
propene	0	1.27	-2.21	3.48	-0.0139	0.0396	5.22	3.01	-1.74
1-butene	0	1.38	-2.19	3.57	-0.0143	0.0386	5.22	3.02	-1.64
1-pentene	0	1.66	-2.29	3.95	-0.0142	0.0382	5.22	2.93	-1.27
E-2-pentene	0	1.34	-2.01	3.35	-0.0144	0.0367	5.22	3.21	-1.87
1-hexene	0	1.68	-2.47	4.15	-0.0139	0.0386	5.22	2.75	-1.07
2-methylpropene	0	1.16	-2.27	3.43	-0.0149	0.0368	5.21	2.95	-1.79
s-trans-1,3-butadiene	0	0.61	-3.79	4.40	-0.0106	0.0429	5.23	1.45	-0.84
cyclopentene	0	0.56	-1.87	2.43	-0.0149	0.0409	5.22	3.34	-2.78
ethyne	0	-0.01	-6.12	6.11	-0.0124	0.0815	5.26	-0.86	0.85
propyne	0	-0.31	-5.06	4.75	-0.0155	0.0770	5.23	0.18	-0.49
1-butyne	0	-0.16	-4.97	4.81	-0.0158	0.0770	5.23	0.26	-0.42
1-pentyne	0	0.01	-4.87	4.88	-0.0164	0.0765	5.23	0.35	-0.34
1-hexyne	0	0.29	-5.20	5.49	-0.0158	0.0765	5.23	0.03	0.26

butenyne	0	0.04	-5.92	5.96	-0.0150	0.0798	5.24	-0.68	0.72
benzene	0	-0.87	-4.70	3.83	-0.0033	0.0448	5.24	0.55	-1.42
ethylbenzene	0	-0.80	-4.62	3.82	-0.0047	0.0440	5.24	0.62	-1.42
naphthalene	0	-2.39	-6.68	4.29	-0.0052	0.0452	5.24	-1.44	-0.95
anthracene	0	-4.23	-8.62	4.39	-0.0054	0.0465	5.24	-3.38	-0.85
toluene	0	-0.89	-4.54	3.65	-0.0047	0.0440	5.24	0.70	-1.59
p-xylene	0	-0.81	-4.36	3.55	-0.0060	0.0416	5.24	0.88	-1.69
m-xylene	0	-0.84	-4.40	3.56	-0.0061	0.0435	5.24	0.84	-1.68
o-xylene	0	-0.90	-4.51	3.61	-0.0056	0.0429	5.24	0.73	-1.63
fluoromethane	0	-0.22	-4.71	4.49	-0.0250	0.0423	5.05	0.34	-0.56
chloromethane	0	-0.56	-4.27	3.71	-0.0104	0.0487	5.24	0.96	-1.52
bromomethane	0	-0.82	-4.22	3.40	-0.0073	0.0500	5.24	1.02	-1.84
chlorofluoromethane	0	-0.77	-6.70	5.93	-0.0155	0.0608	5.22	-1.49	0.72
dichloromethane	0	-1.36	-6.09	4.73	-0.0047	0.0638	5.25	-0.84	-0.52
dibromomethane	0	-2.11	-6.19	4.08	-0.0022	0.0640	5.25	-0.94	-1.17
chlorodifluoromethane	0	-0.50	-6.44	5.94	-0.0081	0.0751	5.26	-1.18	0.68
chloroform	0	-1.07	-5.56	4.49	0.0002	0.0764	5.26	-0.30	-0.77
chloroethane	0	-0.63	-4.28	3.65	-0.0114	0.0464	5.23	0.95	-1.58
bromoethane	0	-0.70	-4.24	3.54	-0.0084	0.0478	5.24	1.00	-1.70
bromoform	0	-1.98	-6.36	4.38	0.0016	0.0748	5.26	-1.10	-0.88
tetrafluoromethane	0	3.16	-2.97	6.13	-0.0003	0.0923	5.29	2.31	0.85
difluorodichloromethane	0	1.69	-2.57	4.26	-0.0017	0.0620	5.25	2.68	-0.99
fluorotrichloromethane	0	0.82	-2.68	3.50	-0.0025	0.0529	5.24	2.56	-1.74
bromotrifluoromethane	0	1.79	-3.23	5.02	-0.0016	0.0907	5.28	2.06	-0.27
bromotrichloromethane	0	-0.93	-3.46	2.53	0.0033	0.0681	5.25	1.79	-2.72
hexafluoroethane	0	3.94	-3.51	7.45	-0.0005	0.0918	5.29	1.77	2.17
hexachloroethane	0	-1.40	-3.67	2.27	0.0038	0.0512	5.24	1.58	-2.98
chloropentafluoroethane	0	2.86	-3.19	6.05	-0.0017	0.0852	5.27	2.09	0.77
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-3.16	4.93	-0.0042	0.0593	5.25	2.09	-0.32
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-7.49	8.01	-0.0097	0.0789	5.26	-2.23	2.75
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-6.89	6.76	-0.0052	0.0781	5.26	-1.62	1.49
1-chloro-2,2,2-trifluoroethane	0	0.06	-7.26	7.32	-0.0074	0.0778	5.26	-1.99	2.05
1,1,1,2-tetrachloroethane	0	-1.15	-6.39	5.24	-0.0047	0.0637	5.25	-1.14	-0.01
1,1,1-trichloroethane	0	-0.25	-4.22	3.97	-0.0020	0.0486	5.24	1.02	-1.27
1,1,2-trichloroethane	0	-1.95	-7.74	5.79	-0.0066	0.0679	5.25	-2.49	0.54

1,1-difluoroethane	0	-0.11	-6.38	6.27	-0.0184	0.0542	5.19	-1.19	1.08
1-bromo-2-chloroethane	0	-1.95	-6.56	4.61	-0.0079	0.0541	5.24	-1.32	-0.63
octafluoropropane	0	4.28	-4.15	8.43	-0.0003	0.0873	5.28	1.13	3.15
2-chloropropane	0	-0.25	-4.30	4.05	-0.0123	0.0450	5.23	0.93	-1.18
1-chloropropane	0	-0.27	-4.27	4.00	-0.0114	0.0457	5.23	0.96	-1.23
1-bromopropane	0	-0.56	-4.26	3.70	-0.0084	0.0471	5.24	0.98	-1.54
2-bromopropane	0	-0.48	-4.26	3.78	-0.0093	0.0466	5.24	0.98	-1.46
2-chlorobutane	0	0.07	-4.14	4.21	-0.0126	0.0444	5.23	1.09	-1.02
1-bromobutane	0	-0.41	-4.34	3.93	-0.0084	0.0470	5.24	0.90	-1.31
1-chloropentane	0	0.07	-4.47	4.54	-0.0115	0.0454	5.23	0.77	-0.70
2-chloropentane	0	0.07	-4.19	4.26	-0.0126	0.0441	5.23	1.03	-0.96
1-bromopentane	0	-0.08	-4.44	4.36	-0.0086	0.0470	5.24	0.80	-0.88
1-bromo-isobutane	0	-0.03	-4.19	4.16	-0.0085	0.0475	5.24	1.05	-1.08
tetrachloroethene	0	0.05	-3.14	3.19	0.0031	0.0498	5.24	2.10	-2.05
trichloroethene	0	-0.39	-4.28	3.89	-0.0005	0.0717	5.26	0.97	-1.36
chloroethene	0	-0.59	-4.00	3.41	-0.0072	0.0581	5.24	1.24	-1.83
E-1,2-dichloroethene	0	-0.76	-4.67	3.91	-0.0038	0.0656	5.25	0.58	-1.34
Z-1,2-dichloroethene	0	-1.17	-5.50	4.33	-0.0033	0.0666	5.25	-0.25	-0.92
3-chloropropene	0	-0.57	-5.29	4.72	-0.0105	0.0498	5.24	-0.05	-0.52
3-bromopropene	0	-0.86	-5.82	4.96	-0.0083	0.0516	5.24	-0.58	-0.28
fluorobenzene	0	-0.78	-5.59	4.81	-0.0186	0.0517	5.18	-0.40	-0.38
chlorobenzene	0	-1.12	-5.24	4.12	-0.0066	0.0516	5.24	0.00	-1.12
bromobenzene	0	-1.46	-5.40	3.94	-0.0044	0.0519	5.24	-0.15	-1.31
1,4-dichlorobenzene	0	-1.01	-5.66	4.65	-0.0052	0.0560	5.24	-0.41	-0.60
1,2-dichlorobenzene	0	-1.36	-5.74	4.38	-0.0056	0.0555	5.24	-0.50	-0.86
p-dibromobenzene	0	-2.30	-5.98	3.68	-0.0028	0.0557	5.24	-0.74	-1.56
chlorotoluene	0	-1.92	-8.15	6.23	-0.0114	0.0500	5.23	-2.92	1.00
o-chlorotoluene	0	-1.15	-4.89	3.74	-0.0076	0.0514	5.24	0.35	-1.50
bromotoluene	0	-2.37	-8.15	5.78	-0.0085	0.0519	5.24	-2.91	0.54
p-bromotoluene	0	-1.39	-5.28	3.89	-0.0049	0.0515	5.24	-0.03	-1.36
2,3-dichlorobiphenyl	0	-2.45	-8.40	5.95	-0.0074	0.0546	5.24	-3.16	0.71
2,2'-dichlorobiphenyl	0	-2.73	-8.94	6.21	-0.0077	0.0513	5.24	-3.70	0.97
2,2',3'-trichlorobiphenyl	0	-1.99	-8.94	6.95	-0.0087	0.0551	5.24	-3.70	1.71
1,2-dimethoxyethane	0	-4.84	-7.46	2.62	-0.0371	0.0356	4.31	-3.15	-1.69
anisole	0	-2.45	-7.32	4.87	-0.0328	0.0470	4.67	-2.64	0.19

dimethyl ether	0	-1.92	-4.85	2.93	-0.0385	0.0358	4.16	-0.69	-1.23
diethyl ether	0	-1.76	-4.98	3.22	-0.0396	0.0331	4.03	-0.95	-0.81
isopropyl ether	0	-0.53	-4.87	4.34	-0.0399	0.0335	3.99	-0.88	0.35
methyl propyl ether	0	-1.66	-4.68	3.02	-0.0383	0.0351	4.18	-0.51	-1.15
methyl isopropyl ether	0	-2.01	-4.72	2.71	-0.0389	0.0344	4.12	-0.60	-1.41
t-butyl methyl ether	0	-2.21	-4.75	2.54	-0.0391	0.0337	4.09	-0.65	-1.56
ethyl phenyl ether	0	-2.22	-7.15	4.93	-0.0330	0.0469	4.66	-2.48	0.26
tetrahydrofuran	0	-3.47	-5.36	1.89	-0.0405	0.0353	3.91	-1.45	-2.02
tetrahydropyran	0	-3.12	-4.92	1.80	-0.0399	0.0336	3.99	-0.93	-2.19
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-8.91	8.79	-0.0241	0.0788	5.10	-3.81	3.69
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-11.06	11.17	-0.0157	0.0788	5.23	-5.82	5.93
acetaldehyde	0	-3.50	-9.28	5.78	-0.0385	0.0576	4.17	-5.12	1.62
propanal	0	-3.44	-8.82	5.38	-0.0386	0.0552	4.15	-4.67	1.23
butanal	0	-3.18	-9.06	5.88	-0.0386	0.0559	4.16	-4.90	1.72
pentanal	0	-3.03	-8.96	5.93	-0.0389	0.0543	4.12	-4.84	1.81
octanal	0	-2.29	-8.74	6.45	-0.0383	0.0479	4.18	-4.56	2.27
benzaldehyde	0	-4.02	-11.05	7.03	-0.0392	0.0534	4.09	-6.96	2.94
p-hydroxybenzaldehyde	0	-10.48	-19.09	8.61	-0.0402	0.1317	4.16	-14.94	4.46
m-hydroxybenzaldehyde	0	-9.51	-18.46	8.95	-0.0390	0.1319	4.30	-14.16	4.65
acetone	0	-3.85	-9.44	5.59	-0.0402	0.0548	3.96	-5.48	1.63
2-butanone	0	-3.64	-8.95	5.31	-0.0407	0.0534	3.90	-5.05	1.41
2-pentanone	0	-3.53	-8.99	5.46	-0.0405	0.0531	3.92	-5.07	1.54
3-pentanone	0	-3.41	-8.46	5.05	-0.0389	0.0525	4.12	-4.34	0.93
2-hexanone	0	-3.29	-9.12	5.83	-0.0405	0.0528	3.92	-5.19	1.90
2-heptanone	0	-3.04	-9.11	6.07	-0.0404	0.0531	3.94	-5.17	2.13
4-heptanone	0	-2.93	-8.57	5.64	-0.0392	0.0524	4.09	-4.48	1.55
2-octanone	0	-2.88	-9.08	6.20	-0.0403	0.0491	3.95	-5.14	2.26
5-nonanone	0	-2.67	-8.68	6.01	-0.0392	0.0520	4.08	-4.60	1.93
3,3-dimethylbutanone	0	-2.89	-8.65	5.76	-0.0407	0.0495	3.89	-4.77	1.88
cyclopentanone	0	-4.68	-9.42	4.74	-0.0403	0.0531	3.95	-5.47	0.79
acetophenone	0	-4.58	-10.92	6.34	-0.0405	0.0518	3.92	-7.00	2.42
methyl formate	0	-2.78	-9.88	7.10	-0.0353	0.0641	4.49	-5.39	2.61
ethyl formate	0	-2.65	-9.76	7.11	-0.0358	0.0641	4.44	-5.31	2.66
methyl acetate	0	-3.32	-9.31	5.99	-0.0374	0.0624	4.29	-5.02	1.70
ethyl acetate	0	-3.10	-9.25	6.15	-0.0378	0.0608	4.24	-5.01	1.91

propyl acetate	0	-2.86	-9.27	6.41	-0.0380	0.0619	4.23	-5.04	2.18
butyl acetate	0	-2.55	-9.29	6.74	-0.0377	0.0600	4.25	-5.04	2.49
methyl propanoate	0	-2.93	-8.98	6.05	-0.0370	0.0612	4.33	-4.65	1.72
methyl butanoate	0	-2.83	-9.03	6.20	-0.0373	0.0612	4.30	-4.73	1.90
methyl pentanoate	0	-2.57	-9.09	6.52	-0.0369	0.0601	4.34	-4.76	2.19
methyl hexanoate	0	-2.49	-9.18	6.69	-0.0374	0.0593	4.29	-4.89	2.40
methyl benzoate	0	-3.91	-10.26	6.35	-0.0378	0.0596	4.24	-6.02	2.11
hydrogen	0	2.33	-0.21	2.54	0.0065	0.0290	5.24	5.03	-2.70
water	0	-6.31	-13.25	6.94	-0.0390	0.1165	4.22	-9.03	2.72
water dimer	0	-11.27	-20.57	9.30	-0.0435	0.1233	3.64	-16.93	5.66
hydrogen peroxide	0	-8.58	-15.15	6.57	-0.0311	0.1307	4.97	-10.17	1.59
methyl peroxide	0	-5.28	-11.11	5.83	-0.0319	0.1299	4.92	-6.20	0.92
ethyl peroxide	0	-5.32	-11.09	5.77	-0.0323	0.1280	4.88	-6.21	0.89
1,4-dioxane	0	-5.05	-8.69	3.64	-0.0378	0.0398	4.24	-4.45	-0.60
methanol	0	-5.11	-9.11	4.00	-0.0391	0.1127	4.19	-4.92	-0.19
ethanol	0	-5.01	-8.79	3.78	-0.0391	0.1127	4.20	-4.59	-0.42
1-propanol	0	-4.83	-8.81	3.98	-0.0390	0.1115	4.21	-4.61	-0.22
isopropanol	0	-4.76	-8.77	4.01	-0.0398	0.1083	4.09	-4.68	-0.08
1-butanol	0	-4.72	-8.92	4.20	-0.0390	0.1113	4.21	-4.71	-0.01
t-butanol	0	-4.51	-8.57	4.06	-0.0394	0.1079	4.14	-4.43	-0.08
1-pentanol	0	-4.47	-9.15	4.68	-0.0395	0.1086	4.13	-5.02	0.55
1-hexanol	0	-4.36	-8.89	4.53	-0.0397	0.1092	4.11	-4.78	0.42
1-heptanol	0	-4.24	-8.44	4.20	-0.0397	0.1061	4.11	-4.33	0.09
1-octanol	0	-4.09	-8.75	4.66	-0.0393	0.1054	4.15	-4.61	0.52
allyl alcohol	0	-5.08	-9.65	4.57	-0.0388	0.1126	4.23	-5.42	0.34
cyclopentanol	0	-5.49	-8.39	2.90	-0.0399	0.1045	4.07	-4.32	-1.17
2-methoxyethanol	0	-6.77	-12.45	5.68	-0.0379	0.1154	4.34	-8.11	1.34
2,2,2-trifluoroethanol	0	-4.31	-14.01	9.70	-0.0304	0.1284	5.00	-9.02	4.71
1,1,1-trifluoropropan-2-ol	0	-4.16	-10.77	6.61	-0.0333	0.1232	4.79	-5.99	1.83
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-13.02	9.25	-0.0259	0.1381	5.26	-7.76	3.99
phenol	0	-6.62	-12.15	5.53	-0.0316	0.1270	4.92	-7.23	0.61
p-bromophenol	0	-7.13	-13.15	6.02	-0.0292	0.1289	5.06	-8.08	0.95
o-cresol	0	-5.87	-11.44	5.57	-0.0317	0.1266	4.91	-6.52	0.65
m-cresol	0	-5.49	-11.94	6.45	-0.0318	0.1287	4.92	-7.03	1.54
p-cresol	0	-6.14	-11.89	5.75	-0.0322	0.1277	4.88	-7.01	0.87

1,2-ethanediol	0	-9.30	-14.93	5.63	-0.0407	0.1208	4.03	-10.90	1.60
acetic acid	0	-6.70	-13.65	6.95	-0.0365	0.1397	4.62	-9.03	2.33
propanoic acid	0	-6.47	-13.31	6.84	-0.0357	0.1395	4.69	-8.62	2.15
butanoic acid	0	-6.36	-13.35	6.99	-0.0357	0.1390	4.69	-8.66	2.30
pentanoic acid	0	-6.16	-13.49	7.33	-0.0357	0.1395	4.69	-8.80	2.64
hexanoic acid	0	-6.21	-13.52	7.31	-0.0358	0.1393	4.68	-8.84	2.63
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-23.03	11.07	-0.0324	0.1452	4.99	-18.04	6.08
ammonia	0	-4.29	-8.32	4.03	-0.0457	0.0691	3.10	-5.22	0.93
methylamine	0	-4.56	-6.52	1.96	-0.0453	0.0666	3.18	-3.34	-1.22
ethylamine	0	-4.50	-6.71	2.21	-0.0455	0.0655	3.15	-3.57	-0.93
butylamine	0	-4.29	-6.84	2.55	-0.0453	0.0653	3.18	-3.66	-0.63
propylamine	0	-4.39	-6.78	2.39	-0.0453	0.0658	3.19	-3.59	-0.80
pentylamine	0	-4.10	-6.98	2.88	-0.0455	0.0650	3.15	-3.83	-0.27
dimethylamine	0	-4.29	-4.87	0.58	-0.0438	0.0659	3.44	-1.43	-2.86
diethylamine	0	-4.07	-4.84	0.77	-0.0437	0.0641	3.45	-1.39	-2.68
dipropylamine	0	-3.66	-4.97	1.31	-0.0434	0.0639	3.51	-1.45	-2.21
trimethylamine	0	-3.23	-3.27	0.04	-0.0421	0.0322	3.70	0.43	-3.66
azetidine	0	-5.56	-5.40	-0.16	-0.0455	0.0654	3.15	-2.25	-3.31
pyrrolidine	0	-5.48	-5.72	0.24	-0.0454	0.0644	3.16	-2.56	-2.92
piperidine	0	-5.11	-4.43	-0.68	-0.0434	0.0658	3.50	-0.93	-4.18
2-methoxyethanamine	0	-6.55	-10.73	4.18	-0.0440	0.0681	3.41	-7.32	0.77
1,2-ethanediamine	0	-9.72	-12.92	3.20	-0.0442	0.0680	3.38	-9.54	-0.18
nitromethane	0	-3.95	-11.96	8.01	-0.0281	0.0617	4.94	-7.02	3.07
nitroethane	0	-3.71	-11.30	7.59	-0.0288	0.0580	4.91	-6.39	2.68
1-nitropropane	0	-3.34	-11.17	7.83	-0.0287	0.0574	4.91	-6.26	2.92
2-nitropropane	0	-3.14	-10.35	7.21	-0.0292	0.0559	4.89	-5.46	2.32
1-nitrobutane	0	-3.08	-11.22	8.14	-0.0289	0.0575	4.90	-6.32	3.24
nitrobenzene	0	-4.12	-10.62	6.50	-0.0278	0.0610	4.96	-5.67	1.55
2-methyl-1-nitrobenzene	0	-3.59	-10.06	6.47	-0.0291	0.0588	4.90	-5.16	1.57
pyridine	0	-4.70	-7.49	2.79	-0.0423	0.0535	3.67	-3.82	-0.88
2-methylpyridine	0	-4.63	-7.03	2.40	-0.0425	0.0516	3.63	-3.39	-1.24
3-methylpyridine	0	-4.77	-7.35	2.58	-0.0428	0.0510	3.60	-3.75	-1.02
4-methylpyridine	0	-4.94	-7.57	2.63	-0.0433	0.0480	3.52	-4.05	-0.89
4-ethylpyridine	0	-4.74	-7.56	2.82	-0.0432	0.0482	3.53	-4.03	-0.71
2,4-dimethylpyridine	0	-4.86	-7.12	2.26	-0.0434	0.0463	3.49	-3.63	-1.23

2,5-dimethylpyridine	0	-4.72	-6.89	2.17	-0.0428	0.0500	3.60	-3.29	-1.43
2,6-dimethylpyridine	0	-4.60	-6.62	2.02	-0.0427	0.0516	3.60	-3.01	-1.59
3,4-dimethylpyridine	0	-5.22	-7.56	2.34	-0.0436	0.0479	3.47	-4.09	-1.13
3,5-dimethylpyridine	0	-4.84	-7.23	2.39	-0.0432	0.0497	3.54	-3.70	-1.14
aniline	0	-5.49	-10.75	5.26	-0.0358	0.0825	4.46	-6.29	0.80
N-methylaniline	0	-4.68	-8.61	3.93	-0.0322	0.0820	4.74	-3.87	-0.81
2-methylaniline	0	-5.56	-10.03	4.47	-0.0365	0.0803	4.39	-5.63	0.07
3-methylaniline	0	-5.67	-10.54	4.87	-0.0363	0.0819	4.41	-6.13	0.46
4-methylaniline	0	-5.55	-10.45	4.90	-0.0366	0.0798	4.38	-6.07	0.52
N-ethylaniline	0	-4.62	-8.44	3.82	-0.0293	0.0841	4.91	-3.53	-1.09
3-aminoaniline	0	-9.92	-16.75	6.83	-0.0360	0.0818	4.44	-12.30	2.38
N,N-dimethylaniline	0	-3.58	-6.51	2.93	-0.0269	0.0432	4.98	-1.52	-2.06
piperazine	0	-7.40	-8.15	0.75	-0.0432	0.0668	3.54	-4.61	-2.79
N-methylpiperazine	0	-7.77	-6.68	-1.09	-0.0429	0.0673	3.58	-3.10	-4.67
N,N'-dimethylpiperazine	0	-7.58	-5.17	-2.41	-0.0412	0.0326	3.82	-1.34	-6.24
1-methylthymine	0	-10.40	-21.23	10.83	-0.0406	0.1178	4.03	-17.20	6.80
9-methyladenine	0	-13.60	-18.85	5.25	-0.0456	0.1011	3.18	-15.68	2.08
acetamide	0	-9.71	-15.79	6.08	-0.0436	0.0993	3.52	-12.27	2.56
E-N-methylacetamide	0	-10.00	-13.87	3.87	-0.0452	0.0937	3.24	-10.63	0.63
Z-N-methylacetamide	0	-10.00	-13.17	3.17	-0.0454	0.1003	3.22	-9.95	-0.05
benzamide	0	-10.90	-16.77	5.87	-0.0432	0.0990	3.59	-13.18	2.28
2,6-dichlorothiobenzamide	0	-10.81	-19.56	8.75	-0.0293	0.1185	5.01	-14.55	3.74
urea	0	-13.80	-20.08	6.28	-0.0428	0.0974	3.65	-16.44	2.64
1,1-dimethyl-3-phenylurea	0	-9.63	-15.50	5.87	-0.0410	0.1006	3.92	-11.58	1.95
hydrazine	0	-6.26	-11.35	5.09	-0.0424	0.0703	3.67	-7.68	1.42
methylhydrazine	0	-5.31	-10.15	4.84	-0.0426	0.0704	3.64	-6.51	1.20
1,1-dimethylhydrazine	0	-4.48	-8.39	3.91	-0.0428	0.0713	3.61	-4.78	0.30
2-methylpyrazine	0	-5.57	-7.95	2.38	-0.0372	0.0528	4.30	-3.65	-1.92
2-ethylpyrazine	0	-5.51	-7.54	2.03	-0.0373	0.0525	4.29	-3.25	-2.26
morpholine	0	-7.17	-8.51	1.34	-0.0417	0.0697	3.77	-4.74	-2.43
N-methylmorpholine	0	-6.34	-6.91	0.57	-0.0400	0.0365	3.98	-2.93	-3.41
acetonitrile	0	-3.89	-9.67	5.78	-0.0336	0.0554	4.62	-5.06	1.17
butanonitrile	0	-3.64	-9.00	5.36	-0.0336	0.0522	4.62	-4.38	0.74
propionitrile	0	-3.85	-9.23	5.38	-0.0338	0.0519	4.61	-4.63	0.78
benzonitrile	0	-4.10	-10.51	6.41	-0.0328	0.0574	4.68	-5.83	1.73

2,6-dichlorobenzonitrile	0	-5.22	-11.01	5.79	-0.0310	0.0620	4.79	-6.21	0.99
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-16.05	7.05	-0.0311	0.1197	4.92	-11.13	2.13
trimethylphosphate	0	-8.70	-15.70	7.00	-0.0418	0.0829	3.78	-11.93	3.23
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-15.82	9.21	-0.0374	0.0916	4.32	-11.50	4.89
phosphine	0	0.60	-1.52	2.12	-0.0130	0.0428	5.23	3.71	-3.11
hydrogen sulfide	0	-0.70	-4.35	3.65	-0.0154	0.0519	5.22	0.87	-1.57
dimethyl sulfide	0	-1.54	-4.45	2.91	-0.0216	0.0415	5.13	0.68	-2.22
diethyl sulfide	0	-1.43	-4.25	2.82	-0.0227	0.0359	5.11	0.86	-2.29
dipropyl sulfide	0	-1.27	-4.46	3.19	-0.0228	0.0355	5.11	0.65	-1.92
bis(2-chloroethyl)sulfide	0	-3.92	-9.99	6.07	-0.0165	0.0506	5.21	-4.78	0.86
dimethyl disulfide	0	-1.83	-5.68	3.85	-0.0168	0.0453	5.20	-0.48	-1.35
diethyl disulfide	0	-1.63	-5.17	3.54	-0.0175	0.0422	5.19	0.03	-1.66
methanethiol	0	-1.24	-4.38	3.14	-0.0190	0.0456	5.18	0.79	-2.03
ethanethiol	0	-1.30	-4.34	3.04	-0.0193	0.0445	5.17	0.83	-2.13
1-propanethiol	0	-1.05	-4.42	3.37	-0.0193	0.0444	5.17	0.75	-1.80
thiophene	0	-1.42	-5.45	4.03	-0.0079	0.0573	5.24	-0.20	-1.22
thiophenol	0	-2.55	-7.39	4.84	-0.0145	0.0527	5.22	-2.17	-0.38
thioanisole	0	-2.73	-7.35	4.62	-0.0173	0.0474	5.20	-2.15	-0.58
tetramethylsilane	0	3.04	-2.12	5.16	-0.0017	0.0384	5.24	3.12	-0.08
acetylene	-1	-76.50	-72.33	-4.17	-0.0664	0.0426	-4.33	-76.66	0.16
acetonitrile	-1	-66.60	-64.90	-1.70	-0.0598	0.0172	-1.05	-65.95	-0.65
cyanamide	-1	-72.20	-70.76	-1.44	-0.0616	0.0487	-1.83	-72.59	0.39
aniline	-1	-62.90	-62.18	-0.72	-0.0697	0.0298	-6.33	-68.51	5.61
diphenylamine	-1	-54.60	-55.01	0.41	-0.0631	0.0327	-2.54	-57.56	2.96
hydrogen cyanide	-1	-70.20	-71.05	0.85	-0.0599	-0.0315	-1.07	-72.13	1.93
formic acid	-1	-76.20	-72.63	-3.57	-0.0636	0.0232	-2.81	-75.43	-0.77
acetic acid	-1	-77.60	-72.63	-4.97	-0.0653	0.0254	-3.67	-76.30	-1.30
propanoic acid	-1	-76.20	-70.56	-5.64	-0.0652	0.0261	-3.66	-74.23	-1.97
hexanoic acid	-1	-74.60	-69.96	-4.64	-0.0653	0.0262	-3.69	-73.65	-0.95
acrylic acid	-1	-74.00	-71.34	-2.66	-0.0648	0.0372	-3.41	-74.75	0.75
pyruvic acid	-1	-68.50	-71.38	2.88	-0.0610	0.0487	-1.55	-72.93	4.43
benzoic acid	-1	-71.20	-68.97	-2.23	-0.0639	0.0408	-2.97	-71.94	0.74
methanol	-1	-95.00	-75.79	-19.21	-0.0786	-0.0090	-13.54	-89.33	-5.67
ethanol	-1	-90.70	-73.07	-17.63	-0.0793	0.0157	-14.18	-87.25	-3.45
1-propanol	-1	-88.30	-72.37	-15.93	-0.0793	0.0205	-14.13	-86.50	-1.80

isopropanol	-1	-86.30	-70.57	-15.73	-0.0788	0.0157	-13.67	-84.24	-2.06
2-butanol	-1	-84.20	-66.96	-17.24	-0.0786	0.0151	-13.51	-80.48	-3.72
t-butanol	-1	-82.30	-68.43	-13.87	-0.0780	0.0159	-12.94	-81.37	-0.93
allyl alcohol	-1	-86.60	-72.29	-14.31	-0.0793	0.0272	-14.15	-86.44	-0.16
benzyl alcohol	-1	-85.10	-67.94	-17.16	-0.0777	0.0362	-12.63	-80.57	-4.53
2-methoxyethanol	-1	-89.40	-74.61	-14.79	-0.0789	0.0281	-13.81	-88.42	-0.98
phenol	-1	-71.90	-64.21	-7.69	-0.0692	0.0309	-6.04	-70.25	-1.65
2-methylphenol	-1	-70.20	-62.31	-7.89	-0.0698	0.0288	-6.40	-68.71	-1.49
3-methylphenol	-1	-71.10	-64.20	-6.90	-0.0696	0.0301	-6.27	-70.46	-0.64
4-methylphenol	-1	-72.00	-64.24	-7.76	-0.0702	0.0291	-6.65	-70.89	-1.11
1,2-ethanediol	-1	-85.30	-79.26	-6.04	-0.0790	0.1017	-13.78	-93.04	7.74
3-hydroxyphenol	-1	-73.80	-68.43	-5.37	-0.0682	0.1151	-5.29	-73.72	-0.08
4-hydroxyphenol	-1	-77.60	-70.87	-6.73	-0.0704	0.1094	-6.74	-77.61	0.01
methyl hydroperoxide	-1	-93.20	-78.97	-14.23	-0.0771	0.0166	-12.14	-91.11	-2.09
ethyl hydroperoxide	-1	-89.20	-78.18	-11.02	-0.0773	0.0259	-12.28	-90.46	1.26
acetaldehyde	-1	-76.50	-68.57	-7.93	-0.0703	0.0149	-6.73	-75.30	-1.20
acetone	-1	-76.20	-67.81	-8.39	-0.0708	0.0207	-7.13	-74.95	-1.25
3-pentanone	-1	-73.70	-62.34	-11.36	-0.0698	0.0187	-6.41	-68.76	-4.94
water	-1	-104.70	-89.30	-15.40	-0.0844	0.0283	-19.62	-108.92	4.22
hydrogen peroxide	-1	-97.30	-85.58	-11.72	-0.0768	0.0779	-11.82	-97.41	0.11
hydroperoxyl radical	-1	-83.30	-78.29	-5.01	-0.0659	-0.0459	-4.02	-82.32	-0.98
2-nitrophenol	-1	-60.10	-62.33	2.23	-0.0618	0.0455	-1.94	-64.28	4.18
3-nitrophenol	-1	-61.90	-58.97	-2.93	-0.0655	0.0509	-3.81	-62.78	0.88
4-nitrophenol	-1	-57.80	-56.71	-1.09	-0.0598	0.0483	-1.02	-57.74	-0.06
nitromethane	-1	-76.50	-70.30	-6.20	-0.0622	0.0340	-2.11	-72.42	-4.08
4-nitroaniline	-1	-57.40	-56.49	-0.91	-0.0593	0.0470	-0.82	-57.31	-0.09
acetamide	-1	-80.20	-70.03	-10.17	-0.0663	0.0291	-4.25	-74.28	-5.92
methanethiol	-1	-73.80	-67.98	-5.82	-0.0520	0.0148	1.65	-66.33	-7.47
ethanethiol	-1	-71.80	-66.21	-5.59	-0.0520	0.0218	1.63	-64.58	-7.22
1-propanethiol	-1	-70.50	-66.00	-4.50	-0.0521	0.0237	1.63	-64.37	-6.13
thiophenol	-1	-63.40	-61.65	-1.75	-0.0474	0.0364	2.75	-58.90	-4.50
hydrogen sulfide	-1	-72.10	-68.84	-3.26	-0.0502	0.0055	2.13	-66.72	-5.38
dimethyl sulfoxide	-1	-67.70	-67.05	-0.65	-0.0677	0.0330	-5.06	-72.11	4.41
hydrofluoric acid	-1	-104.40	-93.94	-10.46	-0.0860	-0.0860	-21.68	-115.61	11.21
hydrochloric acid	-1	-74.50	-72.86	-1.64	-0.0477	-0.0477	2.69	-70.17	-4.33

hydrobromic acid	-1	-68.30	-67.71	-0.59	-0.0397	-0.0397	4.02	-63.69	-4.61
chloroform	-1	-54.10	-52.77	-1.33	-0.0478	0.0105	2.67	-50.10	-4.00
trifluoroacetic acid	-1	-59.30	-63.78	4.48	-0.0569	0.0691	0.11	-63.67	4.37
chloroacetic acid	-1	-69.70	-67.60	-2.10	-0.0608	0.0391	-1.45	-69.05	-0.65
dichloroacetic acid	-1	-62.30	-63.10	0.80	-0.0575	0.0502	-0.12	-63.23	0.93
2,2,2-trifluoroethanol	-1	-77.50	-67.41	-10.09	-0.0741	0.0447	-9.56	-76.97	-0.53
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-61.90	-3.60	-0.0688	0.0542	-5.78	-67.68	2.18
2-chlorophenol	-1	-66.10	-61.38	-4.72	-0.0667	0.0388	-4.49	-65.87	-0.23
4-chlorophenol	-1	-66.00	-59.64	-6.36	-0.0671	0.0388	-4.72	-64.36	-1.64
methylamine	1	-76.40	-83.03	6.63	0.0310	0.1408	5.50	-77.53	1.13
n-propylamine	1	-71.50	-78.46	6.96	0.0048	0.1404	5.49	-72.97	1.47
isopropylamine	1	-69.60	-76.89	7.29	0.0059	0.1385	5.48	-71.41	1.81
tert-butylamine	1	-67.30	-74.48	7.18	0.0063	0.1378	5.48	-69.00	1.70
cyclohexanamine	1	-68.70	-73.96	5.26	0.0043	0.1383	5.48	-68.48	-0.22
allylamine	1	-72.00	-79.19	7.19	-0.0157	0.1424	5.48	-73.71	1.71
dimethylamine	1	-68.60	-74.67	6.07	0.0290	0.1361	5.47	-69.20	0.60
diethylamine	1	-63.40	-69.07	5.67	0.0050	0.1316	5.44	-63.63	0.23
di-n-propylamine	1	-60.50	-67.08	6.58	0.0118	0.1317	5.44	-61.65	1.15
diallylamine	1	-61.60	-68.85	7.25	-0.0119	0.1346	5.45	-63.40	1.80
trimethylamine	1	-61.10	-67.35	6.25	0.0279	0.1331	5.45	-61.90	0.80
triethylamine	1	-54.60	-60.11	5.51	0.0065	0.1230	5.39	-54.72	0.12
aniline	1	-72.40	-80.60	8.20	0.0044	0.1474	5.55	-75.05	2.65
2-methylaniline	1	-70.30	-78.40	8.10	0.0012	0.1468	5.55	-72.86	2.56
3-methylaniline	1	-69.60	-78.82	9.22	0.0025	0.1482	5.56	-73.26	3.66
4-methylaniline	1	-69.80	-78.68	8.88	0.0033	0.1474	5.55	-73.13	3.33
3-aminoaniline	1	-65.80	-83.48	17.68	-0.0238	0.1477	5.40	-78.08	12.28
N-methylaniline	1	-62.60	-72.10	9.50	0.0042	0.1405	5.50	-66.61	4.01
N-ethylaniline	1	-62.20	-69.34	7.14	0.0040	0.1384	5.48	-63.85	1.65
N,N-dimethylaniline	1	-57.20	-64.44	7.24	0.0041	0.1351	5.46	-58.98	1.78
4-methyl-N,N-dimethylaniline	1	-55.90	-62.86	6.96	0.0031	0.1340	5.45	-57.41	1.51
N,N-diethylaniline	1	-54.00	-60.08	6.08	0.0035	0.1288	5.42	-54.66	0.66
1-aminonaphthalene	1	-67.40	-78.39	10.99	0.0003	0.1489	5.56	-72.83	5.43
aziridine	1	-70.90	-76.20	5.30	0.0292	0.1432	5.52	-70.69	-0.21
azetidine	1	-67.70	-71.91	4.21	0.0194	0.1352	5.46	-66.45	-1.25
pyrrolidine	1	-66.00	-70.06	4.06	0.0122	0.1350	5.46	-64.60	-1.40

piperidine	1	-64.20	-68.60	4.40	0.0073	0.1366	5.47	-63.14	-1.06
azacycloheptane	1	-63.30	-67.20	3.90	-0.0028	0.1364	5.47	-61.74	-1.56
pyrrole	1	-61.40	-68.80	7.40	0.0127	0.1456	5.54	-63.27	1.87
pyridine	1	-61.10	-67.62	6.52	0.0183	0.1513	5.58	-62.04	0.94
quinoline	1	-56.00	-62.78	6.78	0.0056	0.1439	5.52	-57.25	1.25
piperazine	1	-66.00	-72.51	6.51	-0.0325	0.1371	4.93	-67.58	1.58
acetonitrile	1	-75.30	-78.61	3.31	0.0361	0.2015	6.33	-72.29	-3.01
ammonia	1	-85.20	-93.56	8.36	0.0644	0.1476	5.55	-88.01	2.81
hydrazine	1	-84.60	-93.86	9.26	-0.0176	0.1469	5.50	-88.37	3.77
methanol	1	-93.00	-92.70	-0.30	0.0103	0.2070	6.45	-86.25	-6.75
ethanol	1	-88.40	-87.37	-1.03	-0.0061	0.2056	6.42	-80.95	-7.45
dimethyl ether	1	-79.70	-77.57	-2.13	0.0066	0.1988	6.27	-71.30	-8.40
diethyl ether	1	-71.50	-69.91	-1.59	0.0024	0.1871	6.05	-63.86	-7.64
acetone	1	-77.10	-77.03	-0.07	0.0009	0.1880	6.06	-70.97	-6.13
acetophenone	1	-64.50	-65.87	1.37	-0.0027	0.1643	5.72	-60.15	-4.35
water	1	-110.30	-113.00	2.70	0.0161	0.2222	6.85	-106.15	-4.15
4-methoxyaniline	1	-71.20	-80.90	9.70	-0.0273	0.1448	5.25	-75.64	4.44
4-nitroaniline	1	-75.90	-96.60	20.70	-0.0220	0.1523	5.48	-91.12	15.22
morpholine	1	-69.60	-77.45	7.85	-0.0265	0.1405	5.25	-72.19	2.59
acetamide	1	-73.90	-83.60	9.70	-0.0052	0.1791	5.92	-77.68	3.78
benzamide	1	-67.20	-76.80	9.60	-0.0073	0.1762	5.87	-70.93	3.73
dimethyl sulfide	1	-64.50	-69.85	5.35	0.0221	0.0950	5.29	-64.56	0.06
dimethyl sulfoxide	1	-67.70	-75.01	7.31	-0.0111	0.1713	5.80	-69.21	1.51
3-chloroaniline	1	-74.70	-84.48	9.78	-0.0047	0.1499	5.57	-78.91	4.21
4-chloroaniline	1	-74.10	-84.91	10.81	-0.0026	0.1499	5.57	-79.34	5.24
PEARSON			0.99					1.00	

Table S 4-1

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/6-31+G* method for the cavity surface with constant density = 0.0005 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.14	2.14	-0.0011	0.0108	1.56	1.42	0.58
ethane	0	1.83	-0.13	1.96	-0.0007	0.0091	1.56	1.44	0.39
n-propane	0	1.96	-0.16	2.12	-0.0008	0.0089	1.56	1.41	0.55
n-butane	0	2.08	-0.18	2.26	-0.0009	0.0089	1.56	1.38	0.70
n-pentane	0	2.33	-0.21	2.54	-0.0009	0.0089	1.56	1.36	0.97
n-hexane	0	2.49	-0.23	2.72	-0.0010	0.0088	1.56	1.33	1.16
n-heptane	0	2.62	-0.26	2.88	-0.0010	0.0085	1.56	1.31	1.31
n-octane	0	2.89	-0.28	3.17	-0.0010	0.0086	1.56	1.28	1.61
2-methylpropane	0	2.32	-0.21	2.53	-0.0008	0.0089	1.56	1.35	0.97
2,2-dimethylpropane	0	2.50	-0.27	2.77	-0.0008	0.0089	1.56	1.29	1.21
2-methylpentane	0	2.52	-0.23	2.75	-0.0010	0.0088	1.56	1.33	1.19
2,4-dimethylpentane	0	2.88	-0.30	3.18	-0.0010	0.0092	1.56	1.27	1.61
2,2,4-trimethylpentane	0	2.85	-0.35	3.20	-0.0011	0.0098	1.56	1.22	1.63
cyclopropane	0	0.75	-0.68	1.43	-0.0088	0.0123	1.44	0.76	-0.01
cyclopentane	0	1.20	-0.18	1.38	-0.0009	0.0085	1.56	1.39	-0.19
cyclohexane	0	1.23	-0.14	1.37	-0.0008	0.0078	1.57	1.43	-0.20
methylcyclohexane	0	1.71	-0.19	1.90	-0.0011	0.0085	1.56	1.37	0.34
cis-1,2-dimethylcyclohexane	0	1.58	-0.22	1.80	-0.0012	0.0090	1.56	1.34	0.24
ethene	0	1.27	-0.84	2.11	-0.0097	0.0145	1.39	0.55	0.72
propene	0	1.27	-0.80	2.07	-0.0104	0.0128	1.37	0.57	0.70
1-butene	0	1.38	-0.76	2.14	-0.0106	0.0125	1.36	0.60	0.78
1-pentene	0	1.66	-0.78	2.44	-0.0106	0.0123	1.36	0.57	1.09
E-2-pentene	0	1.34	-0.64	1.98	-0.0101	0.0111	1.39	0.75	0.59
1-hexene	0	1.68	-0.85	2.53	-0.0104	0.0124	1.37	0.52	1.16
2-methylpropene	0	1.16	-0.81	1.97	-0.0108	0.0114	1.35	0.54	0.62
s-trans-1,3-butadiene	0	0.61	-1.37	1.98	-0.0082	0.0149	1.45	0.07	0.54
cyclopentene	0	0.56	-0.60	1.16	-0.0104	0.0127	1.37	0.77	-0.21
ethyne	0	-0.01	-2.51	2.50	-0.0097	0.0329	1.03	-1.48	1.47
propyne	0	-0.31	-2.15	1.84	-0.0115	0.0302	1.02	-1.13	0.82
1-butyne	0	-0.16	-2.02	1.86	-0.0116	0.0302	1.01	-1.01	0.85
1-pentyne	0	0.01	-1.91	1.92	-0.0116	0.0301	1.02	-0.90	0.91
1-hexyne	0	0.29	-2.10	2.39	-0.0117	0.0298	1.02	-1.08	1.37

butenyne	0	0.04	-2.28	2.32	-0.0103	0.0327	1.01	-1.27	1.31
benzene	0	-0.87	-1.73	0.86	-0.0057	0.0147	1.51	-0.22	-0.65
ethylbenzene	0	-0.80	-1.66	0.86	-0.0066	0.0141	1.50	-0.17	-0.63
naphthalene	0	-2.39	-2.42	0.03	-0.0058	0.0152	1.50	-0.92	-1.47
anthracene	0	-4.23	-3.09	-1.14	-0.0058	0.0151	1.50	-1.59	-2.64
toluene	0	-0.89	-1.67	0.78	-0.0066	0.0141	1.50	-0.17	-0.72
p-xylene	0	-0.81	-1.57	0.76	-0.0074	0.0129	1.49	-0.08	-0.73
m-xylene	0	-0.84	-1.59	0.75	-0.0075	0.0135	1.48	-0.11	-0.73
o-xylene	0	-0.90	-1.68	0.78	-0.0074	0.0134	1.48	-0.19	-0.71
fluoromethane	0	-0.22	-2.26	2.04	-0.0165	0.0162	0.76	-1.50	1.28
chloromethane	0	-0.56	-2.08	1.52	-0.0096	0.0202	1.34	-0.74	0.18
bromomethane	0	-0.82	-2.01	1.19	-0.0081	0.0208	1.39	-0.62	-0.20
chlorofluoromethane	0	-0.77	-2.91	2.14	-0.0101	0.0257	1.22	-1.69	0.92
dichloromethane	0	-1.36	-2.69	1.33	-0.0058	0.0277	1.31	-1.38	0.02
dibromomethane	0	-2.11	-2.63	0.52	-0.0048	0.0280	1.32	-1.32	-0.79
chlorodifluoromethane	0	-0.50	-2.40	1.90	-0.0055	0.0318	1.19	-1.21	0.71
chloroform	0	-1.07	-2.10	1.03	-0.0031	0.0335	1.15	-0.95	-0.12
chloroethane	0	-0.63	-2.03	1.40	-0.0101	0.0183	1.34	-0.69	0.06
bromoethane	0	-0.70	-1.97	1.27	-0.0087	0.0191	1.39	-0.58	-0.12
bromoform	0	-1.98	-2.33	0.35	-0.0026	0.0330	1.17	-1.16	-0.82
tetrafluoromethane	0	3.16	-0.53	3.69	-0.0012	0.0295	1.29	0.76	2.40
difluorodichloromethane	0	1.69	-0.54	2.23	-0.0016	0.0202	1.48	0.95	0.74
fluorotrichloromethane	0	0.82	-0.64	1.46	-0.0020	0.0209	1.47	0.83	-0.01
bromotrifluoromethane	0	1.79	-0.69	2.48	-0.0015	0.0288	1.31	0.62	1.17
bromotrichloromethane	0	-0.93	-1.01	0.08	-0.0010	0.0279	1.34	0.33	-1.26
hexafluoroethane	0	3.94	-0.46	4.40	-0.0011	0.0286	1.32	0.85	3.09
hexachloroethane	0	-1.40	-1.15	-0.25	-0.0025	0.0204	1.48	0.33	-1.73
chloropentafluoroethane	0	2.86	-0.52	3.38	-0.0017	0.0276	1.34	0.83	2.03
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-0.76	2.53	-0.0030	0.0213	1.46	0.71	1.06
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-2.50	3.02	-0.0061	0.0334	1.12	-1.37	1.89
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-2.35	2.22	-0.0039	0.0342	1.12	-1.23	1.10
1-chloro-2,2,2-trifluoroethane	0	0.06	-2.82	2.88	-0.0053	0.0287	1.29	-1.53	1.59
1,1,1,2-tetrachloroethane	0	-1.15	-2.41	1.26	-0.0057	0.0275	1.32	-1.09	-0.06
1,1,1-trichloroethane	0	-0.25	-1.73	1.48	-0.0039	0.0205	1.47	-0.26	0.01
1,1,2-trichloroethane	0	-1.95	-3.01	1.06	-0.0062	0.0286	1.28	-1.73	-0.22

1,1-difluoroethane	0	-0.11	-2.78	2.67	-0.0123	0.0206	1.17	-1.61	1.50
1-bromo-2-chloroethane	0	-1.95	-2.59	0.64	-0.0074	0.0224	1.39	-1.21	-0.74
octafluoropropane	0	4.28	-0.51	4.79	-0.0012	0.0285	1.32	0.81	3.47
2-chloropropane	0	-0.25	-1.97	1.72	-0.0106	0.0169	1.33	-0.65	0.40
1-chloropropane	0	-0.27	-2.00	1.73	-0.0102	0.0177	1.34	-0.66	0.39
1-bromopropane	0	-0.56	-1.95	1.39	-0.0088	0.0184	1.40	-0.56	0.00
2-bromopropane	0	-0.48	-1.91	1.43	-0.0091	0.0177	1.39	-0.52	0.04
2-chlorobutane	0	0.07	-1.84	1.91	-0.0107	0.0165	1.32	-0.52	0.59
1-bromobutane	0	-0.41	-1.98	1.57	-0.0088	0.0184	1.39	-0.59	0.18
1-chloropentane	0	0.07	-2.06	2.13	-0.0103	0.0176	1.33	-0.73	0.80
2-chloropentane	0	0.07	-1.83	1.90	-0.0106	0.0162	1.33	-0.50	0.57
1-bromopentane	0	-0.08	-2.01	1.93	-0.0089	0.0183	1.39	-0.62	0.54
1-bromo-isobutane	0	-0.03	-1.81	1.78	-0.0088	0.0184	1.40	-0.42	0.39
tetrachloroethene	0	0.05	-0.84	0.89	-0.0025	0.0196	1.49	0.65	-0.60
trichloroethene	0	-0.39	-1.42	1.03	-0.0043	0.0293	1.29	-0.13	-0.26
chloroethene	0	-0.59	-1.62	1.03	-0.0070	0.0230	1.39	-0.23	-0.36
E-1,2-dichloroethene	0	-0.76	-1.63	0.87	-0.0045	0.0263	1.36	-0.27	-0.49
Z-1,2-dichloroethene	0	-1.17	-2.27	1.10	-0.0062	0.0271	1.32	-0.95	-0.22
3-chloropropene	0	-0.57	-2.28	1.71	-0.0091	0.0202	1.36	-0.92	0.35
3-bromopropene	0	-0.86	-2.48	1.62	-0.0086	0.0209	1.37	-1.10	0.24
fluorobenzene	0	-0.78	-2.12	1.34	-0.0122	0.0182	1.20	-0.91	0.13
chlorobenzene	0	-1.12	-2.00	0.88	-0.0067	0.0182	1.46	-0.54	-0.58
bromobenzene	0	-1.46	-2.05	0.59	-0.0058	0.0181	1.48	-0.57	-0.89
1,4-dichlorobenzene	0	-1.01	-2.06	1.05	-0.0054	0.0209	1.45	-0.61	-0.40
1,2-dichlorobenzene	0	-1.36	-2.24	0.88	-0.0071	0.0205	1.42	-0.82	-0.54
p-dibromobenzene	0	-2.30	-2.14	-0.16	-0.0046	0.0207	1.46	-0.67	-1.63
chlorotoluene	0	-1.92	-3.35	1.43	-0.0103	0.0197	1.31	-2.04	0.12
o-chlorotoluene	0	-1.15	-1.80	0.65	-0.0070	0.0176	1.46	-0.34	-0.81
bromotoluene	0	-2.37	-3.30	0.93	-0.0090	0.0206	1.36	-1.94	-0.43
p-bromotoluene	0	-1.39	-2.04	0.65	-0.0062	0.0176	1.48	-0.57	-0.82
2,3-dichlorobiphenyl	0	-2.45	-3.09	0.64	-0.0071	0.0201	1.43	-1.66	-0.79
2,2'-dichlorobiphenyl	0	-2.73	-3.43	0.70	-0.0078	0.0183	1.43	-2.00	-0.73
2,2',3'-trichlorobiphenyl	0	-1.99	-3.33	1.34	-0.0072	0.0204	1.42	-1.91	-0.08
1,2-dimethoxyethane	0	-4.84	-2.94	-1.90	-0.0227	0.0132	-0.53	-3.47	-1.37
anisole	0	-2.45	-2.88	0.43	-0.0198	0.0162	0.17	-2.72	0.27

dimethyl ether	0	-1.92	-2.13	0.21	-0.0241	0.0131	-0.95	-3.08	1.16
diethyl ether	0	-1.76	-2.05	0.29	-0.0247	0.0116	-1.13	-3.18	1.42
isopropyl ether	0	-0.53	-1.85	1.32	-0.0245	0.0116	-1.09	-2.95	2.42
methyl propyl ether	0	-1.66	-1.90	0.24	-0.0238	0.0125	-0.86	-2.77	1.11
methyl isopropyl ether	0	-2.01	-1.88	-0.13	-0.0240	0.0122	-0.91	-2.78	0.77
t-butyl methyl ether	0	-2.21	-1.84	-0.37	-0.0241	0.0117	-0.93	-2.77	0.56
ethyl phenyl ether	0	-2.22	-2.72	0.50	-0.0197	0.0159	0.20	-2.52	0.30
tetrahydrofuran	0	-3.47	-2.39	-1.08	-0.0254	0.0124	-1.39	-3.78	0.31
tetrahydropyran	0	-3.12	-2.09	-1.03	-0.0249	0.0112	-1.21	-3.30	0.18
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-3.25	3.13	-0.0145	0.0229	0.92	-2.33	2.21
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-3.74	3.85	-0.0095	0.0331	1.03	-2.70	2.81
acetaldehyde	0	-3.50	-3.96	0.46	-0.0234	0.0192	-0.77	-4.73	1.23
propanal	0	-3.44	-3.65	0.21	-0.0236	0.0174	-0.81	-4.46	1.02
butanal	0	-3.18	-3.81	0.63	-0.0235	0.0171	-0.81	-4.62	1.44
pentanal	0	-3.03	-3.68	0.65	-0.0235	0.0172	-0.79	-4.47	1.44
octanal	0	-2.29	-3.74	1.45	-0.0234	0.0168	-0.77	-4.51	2.22
benzaldehyde	0	-4.02	-4.36	0.34	-0.0243	0.0194	-1.06	-5.42	1.40
p-hydroxybenzaldehyde	0	-10.48	-8.15	-2.33	-0.0254	0.0613	-4.06	-12.21	1.73
m-hydroxybenzaldehyde	0	-9.51	-7.68	-1.83	-0.0242	0.0601	-3.49	-11.18	1.67
acetone	0	-3.85	-4.27	0.42	-0.0246	0.0177	-1.15	-5.42	1.57
2-butanone	0	-3.64	-3.92	0.28	-0.0247	0.0174	-1.18	-5.10	1.46
2-pentanone	0	-3.53	-3.92	0.39	-0.0248	0.0173	-1.22	-5.14	1.61
3-pentanone	0	-3.41	-3.57	0.16	-0.0241	0.0157	-0.97	-4.54	1.13
2-hexanone	0	-3.29	-3.96	0.67	-0.0248	0.0173	-1.21	-5.17	1.88
2-heptanone	0	-3.04	-3.98	0.94	-0.0248	0.0172	-1.22	-5.20	2.16
4-heptanone	0	-2.93	-3.58	0.65	-0.0242	0.0154	-1.00	-4.58	1.65
2-octanone	0	-2.88	-4.00	1.12	-0.0248	0.0172	-1.23	-5.22	2.34
5-nonanone	0	-2.67	-3.66	0.99	-0.0242	0.0153	-1.00	-4.66	1.99
3,3-dimethylbutanone	0	-2.89	-3.65	0.76	-0.0248	0.0173	-1.20	-4.85	1.96
cyclopentanone	0	-4.68	-4.23	-0.45	-0.0247	0.0162	-1.19	-5.41	0.73
acetophenone	0	-4.58	-4.50	-0.08	-0.0251	0.0181	-1.34	-5.84	1.26
methyl formate	0	-2.78	-3.79	1.01	-0.0222	0.0223	-0.49	-4.28	1.50
ethyl formate	0	-2.65	-3.71	1.06	-0.0225	0.0216	-0.55	-4.27	1.62
methyl acetate	0	-3.32	-3.77	0.45	-0.0237	0.0181	-0.87	-4.63	1.31
ethyl acetate	0	-3.10	-3.72	0.62	-0.0240	0.0177	-0.95	-4.67	1.57

propyl acetate	0	-2.86	-3.72	0.86	-0.0240	0.0178	-0.95	-4.67	1.81
butyl acetate	0	-2.55	-3.75	1.20	-0.0240	0.0174	-0.96	-4.71	2.16
methyl propanoate	0	-2.93	-3.51	0.58	-0.0234	0.0168	-0.75	-4.26	1.33
methyl butanoate	0	-2.83	-3.53	0.70	-0.0234	0.0169	-0.76	-4.29	1.46
methyl pentanoate	0	-2.57	-3.56	0.99	-0.0234	0.0165	-0.77	-4.33	1.76
methyl hexanoate	0	-2.49	-3.57	1.08	-0.0235	0.0165	-0.78	-4.36	1.87
methyl benzoate	0	-3.91	-3.92	0.01	-0.0234	0.0176	-0.77	-4.70	0.79
hydrogen	0	2.33	-0.07	2.40	-0.0007	0.0097	1.56	1.49	0.84
water	0	-6.31	-6.43	0.12	-0.0253	0.0516	-2.92	-9.35	3.04
water dimer	0	-11.27	-10.31	-0.96	-0.0290	0.0593	-5.30	-15.61	4.34
hydrogen peroxide	0	-8.58	-6.83	-1.75	-0.0202	0.0573	-2.06	-8.89	0.31
methyl peroxide	0	-5.28	-5.04	-0.24	-0.0209	0.0557	-2.03	-7.07	1.79
ethyl peroxide	0	-5.32	-4.96	-0.36	-0.0213	0.0548	-2.02	-6.98	1.66
1,4-dioxane	0	-5.05	-3.55	-1.50	-0.0232	0.0147	-0.69	-4.25	-0.80
methanol	0	-5.11	-4.26	-0.85	-0.0250	0.0491	-2.59	-6.86	1.75
ethanol	0	-5.01	-3.90	-1.11	-0.0247	0.0485	-2.43	-6.33	1.32
1-propanol	0	-4.83	-3.88	-0.95	-0.0247	0.0478	-2.37	-6.25	1.42
isopropanol	0	-4.76	-3.67	-1.09	-0.0253	0.0441	-2.29	-5.96	1.20
1-butanol	0	-4.72	-3.90	-0.82	-0.0247	0.0474	-2.35	-6.25	1.53
t-butanol	0	-4.51	-3.44	-1.07	-0.0249	0.0438	-2.13	-5.57	1.06
1-pentanol	0	-4.47	-4.01	-0.46	-0.0252	0.0461	-2.42	-6.44	1.97
1-hexanol	0	-4.36	-4.02	-0.34	-0.0254	0.0458	-2.45	-6.47	2.11
1-heptanol	0	-4.24	-4.02	-0.22	-0.0254	0.0454	-2.42	-6.43	2.19
1-octanol	0	-4.09	-4.13	0.04	-0.0252	0.0457	-2.38	-6.51	2.42
allyl alcohol	0	-5.08	-3.90	-1.18	-0.0246	0.0467	-2.25	-6.15	1.07
cyclopentanol	0	-5.49	-3.47	-2.02	-0.0253	0.0418	-2.16	-5.63	0.14
2-methoxyethanol	0	-6.77	-5.35	-1.42	-0.0240	0.0498	-2.32	-7.67	0.90
2,2,2-trifluoroethanol	0	-4.31	-6.44	2.13	-0.0192	0.0591	-2.06	-8.50	4.19
1,1,1-trifluoropropan-2-ol	0	-4.16	-4.11	-0.05	-0.0211	0.0518	-1.67	-5.78	1.62
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-4.30	0.53	-0.0165	0.0605	-1.79	-6.09	2.32
phenol	0	-6.62	-4.99	-1.63	-0.0199	0.0562	-1.86	-6.85	0.23
p-bromophenol	0	-7.13	-5.46	-1.67	-0.0185	0.0581	-1.81	-7.27	0.14
o-cresol	0	-5.87	-4.53	-1.34	-0.0191	0.0558	-1.65	-6.18	0.31
m-cresol	0	-5.49	-4.90	-0.59	-0.0203	0.0559	-1.91	-6.81	1.32
p-cresol	0	-6.14	-4.85	-1.29	-0.0205	0.0557	-1.94	-6.79	0.65

1,2-ethanediol	0	-9.30	-6.71	-2.59	-0.0264	0.0541	-3.56	-10.26	0.96
acetic acid	0	-6.70	-5.41	-1.29	-0.0229	0.0597	-3.04	-8.45	1.75
propanoic acid	0	-6.47	-5.15	-1.32	-0.0225	0.0591	-2.86	-8.01	1.54
butanoic acid	0	-6.36	-5.14	-1.22	-0.0226	0.0590	-2.86	-7.99	1.63
pentanoic acid	0	-6.16	-5.17	-0.99	-0.0225	0.0592	-2.86	-8.03	1.87
hexanoic acid	0	-6.21	-5.19	-1.02	-0.0226	0.0585	-2.81	-8.00	1.79
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-9.41	-2.55	-0.0211	0.0603	-2.66	-12.06	0.10
ammonia	0	-4.29	-4.10	-0.19	-0.0285	0.0290	-2.88	-6.98	2.69
methylamine	0	-4.56	-3.08	-1.48	-0.0273	0.0276	-2.35	-5.43	0.87
ethylamine	0	-4.50	-3.07	-1.43	-0.0274	0.0266	-2.36	-5.43	0.93
butylamine	0	-4.29	-3.09	-1.20	-0.0276	0.0265	-2.44	-5.54	1.25
propylamine	0	-4.39	-3.07	-1.32	-0.0275	0.0266	-2.41	-5.48	1.09
pentylamine	0	-4.10	-3.11	-0.99	-0.0277	0.0259	-2.45	-5.56	1.46
dimethylamine	0	-4.29	-2.15	-2.14	-0.0259	0.0274	-1.76	-3.91	-0.38
diethylamine	0	-4.07	-1.98	-2.09	-0.0255	0.0253	-1.59	-3.58	-0.49
dipropylamine	0	-3.66	-2.00	-1.66	-0.0254	0.0252	-1.56	-3.56	-0.10
trimethylamine	0	-3.23	-1.28	-1.95	-0.0240	0.0110	-0.92	-2.19	-1.04
azetidine	0	-5.56	-2.39	-3.17	-0.0268	0.0265	-2.08	-4.47	-1.09
pyrrolidine	0	-5.48	-2.57	-2.91	-0.0268	0.0260	-2.10	-4.67	-0.81
piperidine	0	-5.11	-1.73	-3.38	-0.0250	0.0269	-1.43	-3.17	-1.94
2-methoxyethanamine	0	-6.55	-4.73	-1.82	-0.0266	0.0287	-2.09	-6.82	0.27
1,2-ethanediamine	0	-9.72	-5.93	-3.79	-0.0267	0.0282	-2.11	-8.05	-1.67
nitromethane	0	-3.95	-5.42	1.47	-0.0183	0.0271	0.29	-5.13	1.18
nitroethane	0	-3.71	-5.08	1.37	-0.0189	0.0243	0.25	-4.84	1.13
1-nitropropane	0	-3.34	-5.00	1.66	-0.0189	0.0237	0.25	-4.74	1.40
2-nitropropane	0	-3.14	-4.61	1.47	-0.0192	0.0222	0.22	-4.39	1.25
1-nitrobutane	0	-3.08	-5.00	1.92	-0.0189	0.0236	0.25	-4.76	1.68
nitrobenzene	0	-4.12	-4.71	0.59	-0.0190	0.0212	0.28	-4.43	0.31
2-methyl-1-nitrobenzene	0	-3.59	-4.48	0.89	-0.0198	0.0202	0.12	-4.35	0.76
pyridine	0	-4.70	-3.27	-1.43	-0.0258	0.0195	-1.61	-4.88	0.18
2-methylpyridine	0	-4.63	-2.90	-1.73	-0.0256	0.0184	-1.50	-4.40	-0.23
3-methylpyridine	0	-4.77	-3.30	-1.47	-0.0263	0.0181	-1.76	-5.06	0.29
4-methylpyridine	0	-4.94	-3.39	-1.55	-0.0265	0.0172	-1.82	-5.21	0.27
4-ethylpyridine	0	-4.74	-3.38	-1.36	-0.0265	0.0172	-1.83	-5.21	0.47
2,4-dimethylpyridine	0	-4.86	-3.01	-1.85	-0.0262	0.0163	-1.70	-4.71	-0.15

2,5-dimethylpyridine	0	-4.72	-2.92	-1.80	-0.0259	0.0173	-1.61	-4.53	-0.19
2,6-dimethylpyridine	0	-4.60	-2.56	-2.04	-0.0253	0.0177	-1.38	-3.93	-0.67
3,4-dimethylpyridine	0	-5.22	-3.51	-1.71	-0.0268	0.0167	-1.95	-5.46	0.24
3,5-dimethylpyridine	0	-4.84	-3.34	-1.50	-0.0267	0.0170	-1.89	-5.23	0.39
aniline	0	-5.49	-4.67	-0.82	-0.0209	0.0373	-0.60	-5.27	-0.22
N-methylaniline	0	-4.68	-3.67	-1.01	-0.0180	0.0366	0.01	-3.66	-1.02
2-methylaniline	0	-5.56	-4.21	-1.35	-0.0210	0.0358	-0.58	-4.79	-0.77
3-methylaniline	0	-5.67	-4.53	-1.14	-0.0212	0.0362	-0.65	-5.18	-0.49
4-methylaniline	0	-5.55	-4.48	-1.07	-0.0217	0.0359	-0.74	-5.22	-0.33
N-ethylaniline	0	-4.62	-3.53	-1.09	-0.0159	0.0369	0.33	-3.20	-1.42
3-aminoaniline	0	-9.92	-7.53	-2.39	-0.0214	0.0363	-0.68	-8.21	-1.71
N,N-dimethylaniline	0	-3.58	-2.73	-0.85	-0.0145	0.0153	1.02	-1.71	-1.87
piperazine	0	-7.40	-3.36	-4.04	-0.0247	0.0276	-1.35	-4.70	-2.70
N-methylpiperazine	0	-7.77	-2.62	-5.15	-0.0245	0.0279	-1.31	-3.93	-3.84
N,N'-dimethylpiperazine	0	-7.58	-1.86	-5.72	-0.0227	0.0110	-0.53	-2.39	-5.19
1-methylthymine	0	-10.40	-9.29	-1.11	-0.0260	0.0512	-3.13	-12.42	2.02
9-methyladenine	0	-13.60	-7.86	-5.74	-0.0244	0.0450	-2.05	-9.91	-3.69
acetamide	0	-9.71	-7.52	-2.19	-0.0273	0.0463	-3.23	-10.75	1.04
E-N-methylacetamide	0	-10.00	-6.75	-3.25	-0.0285	0.0405	-3.37	-10.12	0.12
Z-N-methylacetamide	0	-10.00	-6.43	-3.57	-0.0286	0.0454	-3.72	-10.15	0.15
benzamide	0	-10.90	-7.34	-3.56	-0.0263	0.0447	-2.73	-10.07	-0.83
2,6-dichlorothiobenzamide	0	-10.81	-8.51	-2.30	-0.0170	0.0548	-1.18	-9.69	-1.12
urea	0	-13.80	-9.36	-4.44	-0.0266	0.0447	-2.83	-12.19	-1.61
1,1-dimethyl-3-phenylurea	0	-9.63	-7.07	-2.56	-0.0261	0.0392	-2.30	-9.36	-0.27
hydrazine	0	-6.26	-5.13	-1.13	-0.0255	0.0293	-1.69	-6.82	0.56
methylhydrazine	0	-5.31	-4.68	-0.63	-0.0254	0.0297	-1.67	-6.35	1.04
1,1-dimethylhydrazine	0	-4.48	-3.52	-0.96	-0.0254	0.0297	-1.67	-5.19	0.71
2-methylpyrazine	0	-5.57	-3.39	-2.18	-0.0232	0.0185	-0.72	-4.11	-1.46
2-ethylpyrazine	0	-5.51	-3.10	-2.41	-0.0233	0.0185	-0.74	-3.84	-1.67
morpholine	0	-7.17	-3.59	-3.58	-0.0245	0.0297	-1.35	-4.94	-2.23
N-methylmorpholine	0	-6.34	-2.74	-3.60	-0.0242	0.0128	-0.97	-3.71	-2.63
acetonitrile	0	-3.89	-5.37	1.48	-0.0233	0.0249	-0.84	-6.21	2.32
butanonitrile	0	-3.64	-4.84	1.20	-0.0234	0.0222	-0.83	-5.67	2.03
propionitrile	0	-3.85	-5.05	1.20	-0.0235	0.0223	-0.85	-5.90	2.05
benzonitrile	0	-4.10	-5.04	0.94	-0.0230	0.0225	-0.72	-5.76	1.66

2,6-dichlorobenzonitrile	0	-5.22	-5.34	0.12	-0.0221	0.0251	-0.51	-5.85	0.63
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-6.41	-2.59	-0.0219	0.0478	-1.53	-7.93	-1.07
trimethylphosphate	0	-8.70	-6.63	-2.07	-0.0264	0.0186	-1.80	-8.43	-0.27
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-5.78	-0.83	-0.0233	0.0265	-0.87	-6.66	0.05
phosphine	0	0.60	-0.67	1.27	-0.0113	0.0145	1.30	0.63	-0.03
hydrogen sulfide	0	-0.70	-2.12	1.42	-0.0123	0.0214	1.15	-0.97	0.27
dimethyl sulfide	0	-1.54	-2.05	0.51	-0.0149	0.0164	0.96	-1.08	-0.46
diethyl sulfide	0	-1.43	-1.82	0.39	-0.0152	0.0127	0.95	-0.88	-0.55
dipropyl sulfide	0	-1.27	-1.89	0.62	-0.0154	0.0123	0.93	-0.95	-0.32
bis(2-chloroethyl)sulfide	0	-3.92	-4.00	0.08	-0.0108	0.0204	1.28	-2.72	-1.20
dimethyl disulfide	0	-1.83	-2.45	0.62	-0.0121	0.0184	1.21	-1.24	-0.59
diethyl disulfide	0	-1.63	-2.12	0.49	-0.0124	0.0166	1.21	-0.91	-0.72
methanethiol	0	-1.24	-2.11	0.87	-0.0140	0.0178	1.05	-1.06	-0.18
ethanethiol	0	-1.30	-2.00	0.70	-0.0140	0.0169	1.05	-0.95	-0.35
1-propanethiol	0	-1.05	-2.02	0.97	-0.0140	0.0168	1.05	-0.96	-0.09
thiophene	0	-1.42	-2.00	0.58	-0.0072	0.0215	1.41	-0.59	-0.83
thiophenol	0	-2.55	-2.90	0.35	-0.0109	0.0212	1.26	-1.64	-0.91
thioanisole	0	-2.73	-2.93	0.20	-0.0118	0.0193	1.22	-1.70	-1.03
tetramethylsilane	0	3.04	-0.58	3.62	-0.0039	0.0104	1.55	0.97	2.07
acetylene	-1	-76.50	-60.35	-16.15	-0.0440	0.0016	-14.62	-74.97	-1.53
acetonitrile	-1	-66.60	-56.19	-10.41	-0.0439	-0.0056	-14.46	-70.65	4.05
cyanamide	-1	-72.20	-59.92	-12.28	-0.0445	0.0078	-15.13	-75.06	2.86
aniline	-1	-62.90	-51.16	-11.74	-0.0452	0.0001	-16.03	-67.18	4.28
diphenylamine	-1	-54.60	-44.51	-10.09	-0.0385	0.0034	-9.14	-53.65	-0.95
hydrogen cyanide	-1	-70.20	-61.44	-8.76	-0.0436	-0.0330	-14.14	-75.58	5.38
formic acid	-1	-76.20	-61.06	-15.14	-0.0450	-0.0133	-15.72	-76.78	0.58
acetic acid	-1	-77.60	-59.93	-17.67	-0.0460	-0.0006	-16.95	-76.88	-0.72
propanoic acid	-1	-76.20	-58.09	-18.11	-0.0459	0.0019	-16.88	-74.97	-1.23
hexanoic acid	-1	-74.60	-57.11	-17.49	-0.0458	0.0074	-16.77	-73.88	-0.72
acrylic acid	-1	-74.00	-58.61	-15.39	-0.0456	0.0055	-16.41	-75.03	1.03
pyruvic acid	-1	-68.50	-57.54	-10.96	-0.0436	0.0074	-14.18	-71.71	3.21
benzoic acid	-1	-71.20	-55.87	-15.33	-0.0449	0.0089	-15.68	-71.55	0.35
methanol	-1	-95.00	-63.12	-31.88	-0.0545	-0.0188	-29.84	-92.96	-2.04
ethanol	-1	-90.70	-59.38	-31.32	-0.0538	-0.0060	-28.57	-87.95	-2.75
1-propanol	-1	-88.30	-58.60	-29.70	-0.0539	0.0001	-28.66	-87.26	-1.04

isopropanol	-1	-86.30	-56.38	-29.92	-0.0531	-0.0054	-27.38	-83.76	-2.54
2-butanol	-1	-84.20	-53.95	-30.25	-0.0523	-0.0044	-26.05	-80.00	-4.20
t-butanol	-1	-82.30	-54.03	-28.27	-0.0526	-0.0047	-26.52	-80.55	-1.75
allyl alcohol	-1	-86.60	-58.14	-28.46	-0.0530	0.0007	-27.15	-85.29	-1.31
benzyl alcohol	-1	-85.10	-54.34	-30.76	-0.0517	0.0059	-25.13	-79.47	-5.63
2-methoxyethanol	-1	-89.40	-59.73	-29.67	-0.0535	0.0051	-28.05	-87.78	-1.62
phenol	-1	-71.90	-52.98	-18.92	-0.0469	0.0007	-18.14	-71.12	-0.78
2-methylphenol	-1	-70.20	-51.21	-18.99	-0.0467	0.0001	-17.88	-69.09	-1.11
3-methylphenol	-1	-71.10	-52.65	-18.45	-0.0471	0.0042	-18.43	-71.08	-0.02
4-methylphenol	-1	-72.00	-52.66	-19.34	-0.0474	0.0037	-18.82	-71.48	-0.52
1,2-ethanediol	-1	-85.30	-62.40	-22.90	-0.0537	0.0363	-28.90	-91.31	6.01
3-hydroxyphenol	-1	-73.80	-54.15	-19.65	-0.0462	0.0414	-17.98	-72.13	-1.67
4-hydroxyphenol	-1	-77.60	-55.41	-22.19	-0.0475	0.0408	-19.69	-75.10	-2.50
methyl hydroperoxide	-1	-93.20	-64.41	-28.79	-0.0514	-0.0043	-24.59	-89.00	-4.20
ethyl hydroperoxide	-1	-89.20	-63.42	-25.78	-0.0516	0.0027	-24.87	-88.29	-0.91
acetaldehyde	-1	-76.50	-57.84	-18.66	-0.0484	-0.0073	-20.08	-77.92	1.42
acetone	-1	-76.20	-56.08	-20.12	-0.0484	-0.0028	-20.10	-76.18	-0.02
3-pentanone	-1	-73.70	-51.73	-21.97	-0.0477	-0.0009	-19.16	-70.89	-2.81
water	-1	-104.70	-71.01	-33.69	-0.0582	-0.0087	-36.81	-107.82	3.12
hydrogen peroxide	-1	-97.30	-69.44	-27.86	-0.0518	0.0194	-25.25	-94.69	-2.61
hydroperoxyl radical	-1	-83.30	-67.32	-15.98	-0.0478	-0.0407	-19.35	-86.67	3.37
2-nitrophenol	-1	-60.10	-51.15	-8.95	-0.0424	0.0076	-12.81	-63.96	3.86
3-nitrophenol	-1	-61.90	-48.08	-13.82	-0.0436	0.0111	-14.17	-62.25	0.35
4-nitrophenol	-1	-57.80	-46.76	-11.04	-0.0397	0.0072	-10.20	-56.97	-0.83
nitromethane	-1	-76.50	-58.84	-17.66	-0.0442	0.0003	-14.77	-73.62	-2.88
4-nitroaniline	-1	-57.40	-46.70	-10.70	-0.0384	0.0087	-8.99	-55.70	-1.70
acetamide	-1	-80.20	-57.52	-22.68	-0.0461	-0.0022	-17.03	-74.55	-5.65
methanethiol	-1	-73.80	-56.70	-17.10	-0.0365	-0.0044	-7.47	-64.17	-9.63
ethanethiol	-1	-71.80	-54.36	-17.44	-0.0361	-0.0020	-7.14	-61.50	-10.30
1-propanethiol	-1	-70.50	-54.03	-16.47	-0.0361	0.0036	-7.17	-61.20	-9.30
thiophenol	-1	-63.40	-50.30	-13.10	-0.0329	0.0052	-5.01	-55.31	-8.09
hydrogen sulfide	-1	-72.10	-58.26	-13.84	-0.0367	-0.0118	-7.59	-65.85	-6.25
dimethyl sulfoxide	-1	-67.70	-54.16	-13.54	-0.0463	0.0022	-17.33	-71.50	3.80
hydrofluoric acid	-1	-104.40	-76.25	-28.15	-0.0584	-0.0584	-37.20	-113.45	9.05
hydrochloric acid	-1	-74.50	-62.14	-12.36	-0.0380	-0.0380	-8.68	-70.82	-3.68

hydrobromic acid	-1	-68.30	-58.68	-9.62	-0.0337	-0.0337	-5.46	-64.15	-4.15
chloroform	-1	-54.10	-48.41	-5.69	-0.0330	-0.0117	-5.06	-53.47	-0.63
trifluoroacetic acid	-1	-59.30	-54.41	-4.89	-0.0412	0.0118	-11.62	-66.03	6.73
chloroacetic acid	-1	-69.70	-55.47	-14.23	-0.0429	0.0066	-13.32	-68.79	-0.91
dichloroacetic acid	-1	-62.30	-52.56	-9.74	-0.0407	0.0112	-11.16	-63.72	1.42
2,2,2-trifluoroethanol	-1	-77.50	-56.48	-21.02	-0.0507	-0.0026	-23.41	-79.90	2.40
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-52.02	-13.48	-0.0472	0.0022	-18.50	-70.52	5.02
2-chlorophenol	-1	-66.10	-50.95	-15.15	-0.0451	0.0046	-15.87	-66.82	0.72
4-chlorophenol	-1	-66.00	-49.53	-16.47	-0.0455	0.0046	-16.30	-65.83	-0.17
methylamine	1	-76.40	-70.10	-6.30	0.0244	0.0846	-5.74	-75.83	-0.57
n-propylamine	1	-71.50	-64.93	-6.57	0.0069	0.0839	-5.54	-70.47	-1.03
isopropylamine	1	-69.60	-63.08	-6.52	0.0121	0.0812	-4.85	-67.93	-1.67
tert-butylamine	1	-67.30	-60.22	-7.08	0.0120	0.0790	-4.34	-64.56	-2.74
cyclohexanamine	1	-68.70	-60.00	-8.70	0.0076	0.0802	-4.62	-64.63	-4.07
allylamine	1	-72.00	-64.88	-7.12	-0.0004	0.0840	-5.56	-70.44	-1.56
dimethylamine	1	-68.60	-62.68	-5.92	0.0221	0.0794	-4.43	-67.11	-1.49
diethylamine	1	-63.40	-56.36	-7.04	0.0118	0.0729	-3.02	-59.39	-4.01
di-n-propylamine	1	-60.50	-54.03	-6.47	0.0077	0.0726	-2.98	-57.01	-3.49
diallylamine	1	-61.60	-54.27	-7.33	0.0008	0.0742	-3.29	-57.56	-4.04
trimethylamine	1	-61.10	-56.39	-4.71	0.0214	0.0751	-3.47	-59.86	-1.24
triethylamine	1	-54.60	-48.63	-5.97	0.0109	0.0620	-1.21	-49.85	-4.75
aniline	1	-72.40	-63.63	-8.77	0.0022	0.0864	-6.23	-69.86	-2.54
2-methylaniline	1	-70.30	-61.21	-9.09	0.0014	0.0839	-5.54	-66.75	-3.55
3-methylaniline	1	-69.60	-62.04	-7.56	0.0011	0.0853	-5.93	-67.97	-1.63
4-methylaniline	1	-69.80	-61.87	-7.93	0.0021	0.0851	-5.87	-67.74	-2.06
3-aminoaniline	1	-65.80	-63.28	-2.52	-0.0107	0.0843	-5.85	-69.13	3.33
N-methylaniline	1	-62.60	-56.46	-6.14	0.0018	0.0791	-4.36	-60.82	-1.78
N-ethylaniline	1	-62.20	-53.51	-8.69	0.0019	0.0758	-3.63	-57.14	-5.06
N,N-dimethylaniline	1	-57.20	-50.66	-6.54	0.0018	0.0723	-2.92	-53.58	-3.62
4-methyl-N,N-dimethylaniline	1	-55.90	-49.24	-6.66	0.0017	0.0714	-2.75	-51.99	-3.91
N,N-diethylaniline	1	-54.00	-46.50	-7.50	0.0007	0.0653	-1.70	-48.20	-5.80
1-aminonaphthalene	1	-67.40	-59.92	-7.48	0.0001	0.0870	-6.40	-66.31	-1.09
aziridine	1	-70.90	-64.64	-6.26	0.0229	0.0851	-5.86	-70.50	-0.40
azetidine	1	-67.70	-60.93	-6.77	0.0168	0.0791	-4.36	-65.29	-2.41
pyrrolidine	1	-66.00	-58.59	-7.41	0.0131	0.0780	-4.09	-62.69	-3.31

piperidine	1	-64.20	-56.57	-7.63	0.0118	0.0776	-4.02	-60.59	-3.61
azacycloheptane	1	-63.30	-54.92	-8.38	0.0106	0.0776	-4.02	-58.94	-4.36
pyrrole	1	-61.40	-56.94	-4.46	0.0132	0.0816	-4.97	-61.90	0.50
pyridine	1	-61.10	-55.31	-5.79	0.0154	0.0831	-5.34	-60.65	-0.45
quinoline	1	-56.00	-49.35	-6.65	0.0056	0.0767	-3.83	-53.18	-2.82
piperazine	1	-66.00	-58.18	-7.82	-0.0136	0.0783	-4.61	-62.79	-3.21
acetonitrile	1	-75.30	-64.27	-11.03	0.0287	0.1109	-15.30	-79.57	4.27
ammonia	1	-85.20	-79.27	-5.93	0.0503	0.0910	-7.57	-86.84	1.64
hydrazine	1	-84.60	-76.96	-7.64	-0.0050	0.0888	-6.92	-83.88	-0.72
methanol	1	-93.00	-76.09	-16.91	0.0150	0.1216	-20.92	-97.01	4.01
ethanol	1	-88.40	-70.50	-17.90	0.0124	0.1189	-19.38	-89.89	1.49
dimethyl ether	1	-79.70	-64.09	-15.61	0.0123	0.1133	-16.49	-80.58	0.88
diethyl ether	1	-71.50	-55.97	-15.53	0.0083	0.0991	-10.35	-66.31	-5.19
acetone	1	-77.10	-61.01	-16.09	0.0074	0.1010	-11.06	-72.07	-5.03
acetophenone	1	-64.50	-50.06	-14.44	0.0033	0.0835	-5.43	-55.49	-9.01
water	1	-110.30	-92.33	-17.97	0.0190	0.1330	-28.13	-120.45	10.15
4-methoxyaniline	1	-71.20	-62.06	-9.14	-0.0135	0.0853	-6.33	-68.39	-2.81
4-nitroaniline	1	-75.90	-74.04	-1.86	-0.0129	0.0913	-8.05	-82.08	6.18
morpholine	1	-69.60	-61.77	-7.83	-0.0119	0.0810	-5.10	-66.87	-2.73
acetamide	1	-73.90	-66.07	-7.83	0.0024	0.0964	-9.36	-75.43	1.53
benzamide	1	-67.20	-57.85	-9.35	0.0020	0.0936	-8.41	-66.27	-0.93
dimethyl sulfide	1	-64.50	-57.90	-6.60	0.0176	0.0533	-0.17	-58.07	-6.43
dimethyl sulfoxide	1	-67.70	-58.84	-8.86	-0.0007	0.0927	-8.12	-66.96	-0.74
3-chloroaniline	1	-74.70	-66.04	-8.66	-0.0022	0.0887	-6.88	-72.92	-1.78
4-chloroaniline	1	-74.10	-66.27	-7.83	-0.0013	0.0884	-6.79	-73.06	-1.04
PEARSON			0.99					1.00	

Table S 4-2

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/6-31+G* method for the cavity surface with constant density = 0.001 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.26	2.26	0.0009	0.0187	2.34	2.08	-0.08
ethane	0	1.83	-0.24	2.07	0.0007	0.0162	2.34	2.10	-0.27
n-propane	0	1.96	-0.29	2.25	0.0007	0.0159	2.34	2.05	-0.09
n-butane	0	2.08	-0.33	2.41	0.0006	0.0160	2.34	2.01	0.07
n-pentane	0	2.33	-0.38	2.71	0.0006	0.0159	2.34	1.96	0.37
n-hexane	0	2.49	-0.42	2.91	0.0006	0.0159	2.34	1.92	0.57
n-heptane	0	2.62	-0.46	3.08	0.0007	0.0155	2.34	1.88	0.74
n-octane	0	2.89	-0.50	3.39	0.0005	0.0154	2.34	1.84	1.05
2-methylpropane	0	2.32	-0.38	2.70	0.0007	0.0160	2.34	1.96	0.36
2,2-dimethylpropane	0	2.50	-0.49	2.99	0.0009	0.0160	2.34	1.85	0.65
2-methylpentane	0	2.52	-0.44	2.96	0.0004	0.0158	2.34	1.91	0.61
2,4-dimethylpentane	0	2.88	-0.54	3.42	0.0006	0.0163	2.34	1.81	1.07
2,2,4-trimethylpentane	0	2.85	-0.62	3.47	-0.0008	0.0164	2.34	1.72	1.13
cyclopropane	0	0.75	-1.08	1.83	-0.0097	0.0206	2.30	1.22	-0.47
cyclopentane	0	1.20	-0.32	1.52	0.0006	0.0154	2.34	2.02	-0.82
cyclohexane	0	1.23	-0.27	1.50	0.0007	0.0144	2.34	2.07	-0.84
methylcyclohexane	0	1.71	-0.36	2.07	0.0005	0.0156	2.34	1.99	-0.28
cis-1,2-dimethylcyclohexane	0	1.58	-0.42	2.00	0.0004	0.0158	2.34	1.92	-0.34
ethene	0	1.27	-1.26	2.53	-0.0108	0.0236	2.28	1.02	0.25
propene	0	1.27	-1.22	2.49	-0.0116	0.0215	2.27	1.05	0.22
1-butene	0	1.38	-1.18	2.56	-0.0119	0.0209	2.27	1.09	0.29
1-pentene	0	1.66	-1.23	2.89	-0.0119	0.0207	2.27	1.04	0.62
E-2-pentene	0	1.34	-1.04	2.38	-0.0115	0.0190	2.28	1.24	0.10
1-hexene	0	1.68	-1.32	3.00	-0.0115	0.0211	2.27	0.95	0.73
2-methylpropene	0	1.16	-1.25	2.41	-0.0122	0.0196	2.26	1.01	0.15
s-trans-1,3-butadiene	0	0.61	-2.02	2.63	-0.0087	0.0240	2.31	0.29	0.32
cyclopentene	0	0.56	-0.95	1.51	-0.0118	0.0214	2.27	1.32	-0.76
ethyne	0	-0.01	-3.59	3.58	-0.0106	0.0485	2.09	-1.49	1.48
propyne	0	-0.31	-3.07	2.76	-0.0130	0.0450	2.09	-0.98	0.67
1-butyne	0	-0.16	-2.94	2.78	-0.0131	0.0451	2.09	-0.85	0.69
1-pentyne	0	0.01	-2.81	2.82	-0.0131	0.0449	2.09	-0.72	0.73
1-hexyne	0	0.29	-3.06	3.35	-0.0133	0.0446	2.09	-0.97	1.26

butenyne	0	0.04	-3.28	3.32	-0.0115	0.0480	2.09	-1.19	1.23
benzene	0	-0.87	-2.44	1.57	-0.0046	0.0239	2.33	-0.12	-0.75
ethylbenzene	0	-0.80	-2.39	1.59	-0.0058	0.0231	2.33	-0.06	-0.74
naphthalene	0	-2.39	-3.39	1.00	-0.0052	0.0244	2.32	-1.07	-1.32
anthracene	0	-4.23	-4.31	0.08	-0.0053	0.0244	2.32	-1.99	-2.24
toluene	0	-0.89	-2.38	1.49	-0.0057	0.0231	2.33	-0.05	-0.84
p-xylene	0	-0.81	-2.28	1.47	-0.0068	0.0215	2.33	0.05	-0.86
m-xylene	0	-0.84	-2.30	1.46	-0.0068	0.0225	2.32	0.02	-0.86
o-xylene	0	-0.90	-2.41	1.51	-0.0067	0.0223	2.32	-0.08	-0.82
fluoromethane	0	-0.22	-2.92	2.70	-0.0187	0.0253	1.97	-0.94	0.72
chloromethane	0	-0.56	-2.76	2.20	-0.0099	0.0305	2.27	-0.49	-0.07
bromomethane	0	-0.82	-2.69	1.87	-0.0080	0.0313	2.29	-0.41	-0.41
chlorofluoromethane	0	-0.77	-3.93	3.16	-0.0112	0.0376	2.21	-1.72	0.95
dichloromethane	0	-1.36	-3.71	2.35	-0.0055	0.0405	2.23	-1.47	0.11
dibromomethane	0	-2.11	-3.71	1.60	-0.0041	0.0408	2.23	-1.48	-0.63
chlorodifluoromethane	0	-0.50	-3.39	2.89	-0.0053	0.0460	2.17	-1.22	0.72
chloroform	0	-1.07	-3.08	2.01	-0.0018	0.0485	2.14	-0.94	-0.13
chloroethane	0	-0.63	-2.71	2.08	-0.0107	0.0282	2.27	-0.44	-0.19
bromoethane	0	-0.70	-2.65	1.95	-0.0087	0.0291	2.29	-0.36	-0.34
bromoform	0	-1.98	-3.49	1.51	-0.0011	0.0478	2.15	-1.34	-0.64
tetrafluoromethane	0	3.16	-0.96	4.12	-0.0002	0.0453	2.18	1.22	1.94
difluorodichloromethane	0	1.69	-0.96	2.65	-0.0006	0.0309	2.30	1.35	0.34
fluorotrichloromethane	0	0.82	-1.11	1.93	-0.0012	0.0318	2.30	1.20	-0.38
bromotrifluoromethane	0	1.79	-1.19	2.98	-0.0006	0.0448	2.19	1.00	0.79
bromotrichloromethane	0	-0.93	-1.62	0.69	0.0007	0.0410	2.23	0.61	-1.54
hexafluoroethane	0	3.94	-0.93	4.87	-0.0002	0.0445	2.19	1.27	2.67
hexachloroethane	0	-1.40	-1.84	0.44	-0.0007	0.0310	2.30	0.47	-1.87
chloropentafluoroethane	0	2.86	-0.96	3.82	-0.0009	0.0426	2.22	1.25	1.61
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.25	3.02	-0.0025	0.0323	2.30	1.04	0.73
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-3.66	4.18	-0.0066	0.0481	2.14	-1.52	2.04
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-3.49	3.36	-0.0034	0.0493	2.13	-1.36	1.23
1-chloro-2,2,2-trifluoroethane	0	0.06	-3.96	4.02	-0.0051	0.0416	2.22	-1.73	1.79
1,1,1,2-tetrachloroethane	0	-1.15	-3.54	2.39	-0.0052	0.0403	2.24	-1.31	0.16
1,1,1-trichloroethane	0	-0.25	-2.47	2.22	-0.0033	0.0309	2.30	-0.16	-0.09
1,1,2-trichloroethane	0	-1.95	-4.38	2.43	-0.0062	0.0420	2.22	-2.16	0.21

1,1-difluoroethane	0	-0.11	-3.71	3.60	-0.0137	0.0313	2.19	-1.52	1.41
1-bromo-2-chloroethane	0	-1.95	-3.76	1.81	-0.0076	0.0335	2.28	-1.48	-0.47
octafluoropropane	0	4.28	-1.04	5.32	-0.0002	0.0439	2.20	1.16	3.12
2-chloropropane	0	-0.25	-2.67	2.42	-0.0112	0.0265	2.27	-0.40	0.15
1-chloropropane	0	-0.27	-2.69	2.42	-0.0107	0.0274	2.27	-0.41	0.14
1-bromopropane	0	-0.56	-2.65	2.09	-0.0088	0.0284	2.29	-0.35	-0.21
2-bromopropane	0	-0.48	-2.60	2.12	-0.0093	0.0275	2.29	-0.31	-0.17
2-chlorobutane	0	0.07	-2.52	2.59	-0.0113	0.0259	2.27	-0.25	0.32
1-bromobutane	0	-0.41	-2.69	2.28	-0.0089	0.0283	2.29	-0.40	-0.01
1-chloropentane	0	0.07	-2.79	2.86	-0.0109	0.0274	2.27	-0.52	0.59
2-chloropentane	0	0.07	-2.52	2.59	-0.0113	0.0256	2.27	-0.25	0.32
1-bromopentane	0	-0.08	-2.73	2.65	-0.0089	0.0283	2.29	-0.44	0.36
1-bromo-isobutane	0	-0.03	-2.51	2.48	-0.0088	0.0282	2.29	-0.21	0.18
tetrachloroethene	0	0.05	-1.39	1.44	-0.0009	0.0299	2.31	0.92	-0.87
trichloroethene	0	-0.39	-2.13	1.74	-0.0024	0.0430	2.21	0.08	-0.47
chloroethene	0	-0.59	-2.27	1.68	-0.0070	0.0346	2.27	0.00	-0.59
E-1,2-dichloroethene	0	-0.76	-2.44	1.68	-0.0042	0.0392	2.25	-0.19	-0.57
Z-1,2-dichloroethene	0	-1.17	-3.12	1.95	-0.0045	0.0401	2.24	-0.88	-0.29
3-chloropropene	0	-0.57	-3.18	2.61	-0.0093	0.0308	2.28	-0.90	0.33
3-bromopropene	0	-0.86	-3.43	2.57	-0.0085	0.0317	2.28	-1.15	0.29
fluorobenzene	0	-0.78	-2.94	2.16	-0.0136	0.0287	2.20	-0.74	-0.04
chlorobenzene	0	-1.12	-2.80	1.68	-0.0066	0.0285	2.31	-0.50	-0.62
bromobenzene	0	-1.46	-2.88	1.42	-0.0053	0.0285	2.31	-0.57	-0.89
1,4-dichlorobenzene	0	-1.01	-2.98	1.97	-0.0052	0.0320	2.30	-0.68	-0.33
1,2-dichlorobenzene	0	-1.36	-3.11	1.75	-0.0062	0.0315	2.30	-0.81	-0.55
p-dibromobenzene	0	-2.30	-3.12	0.82	-0.0040	0.0316	2.30	-0.82	-1.48
chlorotoluene	0	-1.92	-4.60	2.68	-0.0108	0.0302	2.26	-2.34	0.42
o-chlorotoluene	0	-1.15	-2.58	1.43	-0.0070	0.0280	2.31	-0.27	-0.88
bromotoluene	0	-2.37	-4.56	2.19	-0.0090	0.0313	2.28	-2.28	-0.09
p-bromotoluene	0	-1.39	-2.87	1.48	-0.0057	0.0279	2.31	-0.56	-0.83
2,3-dichlorobiphenyl	0	-2.45	-4.36	1.91	-0.0058	0.0310	2.30	-2.06	-0.39
2,2'-dichlorobiphenyl	0	-2.73	-4.79	2.06	-0.0071	0.0287	2.30	-2.49	-0.24
2,2',3'-trichlorobiphenyl	0	-1.99	-4.72	2.73	-0.0074	0.0314	2.29	-2.43	0.44
1,2-dimethoxyethane	0	-4.84	-4.24	-0.60	-0.0271	0.0216	0.99	-3.25	-1.59
anisole	0	-2.45	-4.03	1.58	-0.0235	0.0255	1.53	-2.50	0.05

dimethyl ether	0	-1.92	-2.91	0.99	-0.0285	0.0215	0.73	-2.18	0.26
diethyl ether	0	-1.76	-2.89	1.13	-0.0293	0.0195	0.58	-2.31	0.55
isopropyl ether	0	-0.53	-2.73	2.20	-0.0293	0.0194	0.57	-2.16	1.63
methyl propyl ether	0	-1.66	-2.69	1.03	-0.0283	0.0208	0.78	-1.92	0.26
methyl isopropyl ether	0	-2.01	-2.70	0.69	-0.0285	0.0204	0.73	-1.96	-0.05
t-butyl methyl ether	0	-2.21	-2.69	0.48	-0.0287	0.0198	0.70	-1.99	-0.22
ethyl phenyl ether	0	-2.22	-3.87	1.65	-0.0235	0.0253	1.53	-2.35	0.13
tetrahydrofuran	0	-3.47	-3.23	-0.24	-0.0300	0.0204	0.42	-2.82	-0.65
tetrahydropyran	0	-3.12	-2.89	-0.23	-0.0295	0.0190	0.53	-2.36	-0.76
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-4.65	4.53	-0.0170	0.0346	2.04	-2.62	2.50
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-5.48	5.59	-0.0110	0.0480	2.09	-3.39	3.50
acetaldehyde	0	-3.50	-5.17	1.67	-0.0277	0.0292	0.87	-4.29	0.79
propanal	0	-3.44	-4.82	1.38	-0.0278	0.0267	0.86	-3.95	0.51
butanal	0	-3.18	-5.01	1.83	-0.0278	0.0262	0.87	-4.14	0.96
pentanal	0	-3.03	-4.88	1.85	-0.0279	0.0264	0.83	-4.05	1.02
octanal	0	-2.29	-4.97	2.68	-0.0276	0.0265	0.89	-4.08	1.79
benzaldehyde	0	-4.02	-5.82	1.80	-0.0286	0.0296	0.69	-5.13	1.11
p-hydroxybenzaldehyde	0	-10.48	-10.99	0.51	-0.0300	0.0851	-1.13	-12.12	1.64
m-hydroxybenzaldehyde	0	-9.51	-10.47	0.96	-0.0285	0.0841	-0.74	-11.21	1.70
acetone	0	-3.85	-5.57	1.72	-0.0292	0.0273	0.58	-4.99	1.14
2-butanone	0	-3.64	-5.18	1.54	-0.0294	0.0267	0.54	-4.64	1.00
2-pentanone	0	-3.53	-5.20	1.67	-0.0293	0.0267	0.55	-4.65	1.12
3-pentanone	0	-3.41	-4.79	1.38	-0.0285	0.0243	0.73	-4.06	0.65
2-hexanone	0	-3.29	-5.25	1.96	-0.0293	0.0269	0.54	-4.71	1.42
2-heptanone	0	-3.04	-5.29	2.25	-0.0295	0.0264	0.52	-4.77	1.73
4-heptanone	0	-2.93	-4.83	1.90	-0.0285	0.0241	0.74	-4.09	1.16
2-octanone	0	-2.88	-5.33	2.45	-0.0292	0.0260	0.57	-4.76	1.88
5-nonanone	0	-2.67	-4.92	2.25	-0.0285	0.0237	0.72	-4.20	1.53
3,3-dimethylbutanone	0	-2.89	-4.90	2.01	-0.0295	0.0273	0.50	-4.40	1.51
cyclopentanone	0	-4.68	-5.51	0.83	-0.0293	0.0256	0.56	-4.95	0.27
acetophenone	0	-4.58	-6.04	1.46	-0.0299	0.0278	0.42	-5.62	1.04
methyl formate	0	-2.78	-5.25	2.47	-0.0259	0.0342	1.16	-4.09	1.31
ethyl formate	0	-2.65	-5.15	2.50	-0.0263	0.0332	1.09	-4.07	1.42
methyl acetate	0	-3.32	-5.21	1.89	-0.0278	0.0281	0.85	-4.36	1.04
ethyl acetate	0	-3.10	-5.16	2.06	-0.0281	0.0277	0.79	-4.37	1.27

propyl acetate	0	-2.86	-5.18	2.32	-0.0282	0.0277	0.78	-4.39	1.53
butyl acetate	0	-2.55	-5.24	2.69	-0.0281	0.0275	0.79	-4.44	1.89
methyl propanoate	0	-2.93	-4.92	1.99	-0.0273	0.0267	0.96	-3.97	1.04
methyl butanoate	0	-2.83	-4.96	2.13	-0.0273	0.0264	0.95	-4.01	1.18
methyl pentanoate	0	-2.57	-5.02	2.45	-0.0273	0.0264	0.95	-4.07	1.50
methyl hexanoate	0	-2.49	-5.06	2.57	-0.0273	0.0262	0.95	-4.11	1.62
methyl benzoate	0	-3.91	-5.52	1.61	-0.0274	0.0275	0.93	-4.59	0.68
hydrogen	0	2.33	-0.12	2.45	0.0013	0.0164	2.34	2.23	0.10
water	0	-6.31	-8.66	2.35	-0.0299	0.0732	-0.47	-9.13	2.82
water dimer	0	-11.27	-13.80	2.53	-0.0339	0.0817	-2.00	-15.79	4.52
hydrogen peroxide	0	-8.58	-9.39	0.81	-0.0239	0.0805	0.22	-9.17	0.59
methyl peroxide	0	-5.28	-6.87	1.59	-0.0246	0.0793	0.19	-6.68	1.40
ethyl peroxide	0	-5.32	-6.81	1.49	-0.0250	0.0782	0.20	-6.61	1.29
1,4-dioxane	0	-5.05	-5.00	-0.05	-0.0275	0.0236	0.92	-4.08	-0.97
methanol	0	-5.11	-5.78	0.67	-0.0295	0.0702	-0.25	-6.04	0.93
ethanol	0	-5.01	-5.41	0.40	-0.0293	0.0697	-0.18	-5.59	0.58
1-propanol	0	-4.83	-5.40	0.57	-0.0292	0.0688	-0.12	-5.53	0.70
isopropanol	0	-4.76	-5.20	0.44	-0.0299	0.0649	-0.14	-5.34	0.58
1-butanol	0	-4.72	-5.44	0.72	-0.0293	0.0685	-0.13	-5.57	0.85
t-butanol	0	-4.51	-4.97	0.46	-0.0295	0.0645	-0.04	-5.00	0.49
1-pentanol	0	-4.47	-5.60	1.13	-0.0299	0.0666	-0.21	-5.81	1.34
1-hexanol	0	-4.36	-5.66	1.30	-0.0299	0.0675	-0.24	-5.90	1.54
1-heptanol	0	-4.24	-5.72	1.48	-0.0299	0.0660	-0.18	-5.91	1.67
1-octanol	0	-4.09	-5.63	1.54	-0.0298	0.0669	-0.19	-5.81	1.72
allyl alcohol	0	-5.08	-5.60	0.52	-0.0291	0.0684	-0.08	-5.68	0.60
cyclopentanol	0	-5.49	-4.91	-0.58	-0.0299	0.0619	-0.05	-4.96	-0.53
2-methoxyethanol	0	-6.77	-7.49	0.72	-0.0284	0.0717	-0.08	-7.57	0.80
2,2,2-trifluoroethanol	0	-4.31	-8.53	4.22	-0.0226	0.0820	0.29	-8.24	3.93
1,1,1-trifluoropropan-2-ol	0	-4.16	-5.90	1.74	-0.0249	0.0745	0.40	-5.50	1.34
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-6.43	2.66	-0.0194	0.0848	0.41	-6.02	2.25
phenol	0	-6.62	-7.01	0.39	-0.0232	0.0796	0.35	-6.65	0.03
p-bromophenol	0	-7.13	-7.64	0.51	-0.0216	0.0816	0.42	-7.23	0.10
o-cresol	0	-5.87	-6.49	0.62	-0.0227	0.0792	0.44	-6.05	0.18
m-cresol	0	-5.49	-6.90	1.41	-0.0237	0.0797	0.30	-6.60	1.11
p-cresol	0	-6.14	-6.85	0.71	-0.0238	0.0794	0.30	-6.55	0.41

1,2-ethanediol	0	-9.30	-9.15	-0.15	-0.0309	0.0762	-0.84	-9.99	0.69
acetic acid	0	-6.70	-7.63	0.93	-0.0269	0.0852	-0.52	-8.15	1.45
propanoic acid	0	-6.47	-7.33	0.86	-0.0264	0.0846	-0.39	-7.72	1.25
butanoic acid	0	-6.36	-7.34	0.98	-0.0264	0.0846	-0.39	-7.73	1.37
pentanoic acid	0	-6.16	-7.39	1.23	-0.0262	0.0848	-0.37	-7.76	1.60
hexanoic acid	0	-6.21	-7.43	1.22	-0.0264	0.0841	-0.35	-7.78	1.57
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-13.22	1.26	-0.0237	0.0869	-0.16	-13.38	1.42
ammonia	0	-4.29	-5.60	1.31	-0.0350	0.0432	-1.15	-6.75	2.46
methylamine	0	-4.56	-4.28	-0.28	-0.0339	0.0413	-0.77	-5.06	0.50
ethylamine	0	-4.50	-4.30	-0.20	-0.0339	0.0401	-0.76	-5.06	0.56
butylamine	0	-4.29	-4.35	0.06	-0.0341	0.0398	-0.81	-5.16	0.87
propylamine	0	-4.39	-4.32	-0.07	-0.0341	0.0403	-0.80	-5.12	0.73
pentylamine	0	-4.10	-4.38	0.28	-0.0342	0.0394	-0.84	-5.21	1.11
dimethylamine	0	-4.29	-3.06	-1.23	-0.0322	0.0410	-0.26	-3.32	-0.97
diethylamine	0	-4.07	-2.90	-1.17	-0.0318	0.0386	-0.13	-3.03	-1.04
dipropylamine	0	-3.66	-2.94	-0.72	-0.0317	0.0385	-0.08	-3.02	-0.64
trimethylamine	0	-3.23	-1.89	-1.34	-0.0301	0.0188	0.39	-1.50	-1.73
azetidine	0	-5.56	-3.36	-2.20	-0.0333	0.0400	-0.56	-3.92	-1.64
pyrrolidine	0	-5.48	-3.60	-1.88	-0.0333	0.0394	-0.56	-4.16	-1.32
piperidine	0	-5.11	-2.58	-2.53	-0.0313	0.0404	0.00	-2.58	-2.53
2-methoxyethanamine	0	-6.55	-6.60	0.05	-0.0329	0.0423	-0.48	-7.08	0.53
1,2-ethanediamine	0	-9.72	-8.28	-1.44	-0.0331	0.0422	-0.53	-8.81	-0.91
nitromethane	0	-3.95	-6.98	3.03	-0.0210	0.0392	1.72	-5.27	1.32
nitroethane	0	-3.71	-6.57	2.86	-0.0216	0.0356	1.69	-4.89	1.18
1-nitropropane	0	-3.34	-6.49	3.15	-0.0216	0.0350	1.69	-4.80	1.46
2-nitropropane	0	-3.14	-5.98	2.84	-0.0220	0.0328	1.67	-4.31	1.17
1-nitrobutane	0	-3.08	-6.52	3.44	-0.0217	0.0349	1.69	-4.83	1.75
nitrobenzene	0	-4.12	-6.18	2.06	-0.0216	0.0331	1.70	-4.48	0.36
2-methyl-1-nitrobenzene	0	-3.59	-5.89	2.30	-0.0227	0.0312	1.60	-4.29	0.70
pyridine	0	-4.70	-4.42	-0.28	-0.0315	0.0299	0.01	-4.41	-0.29
2-methylpyridine	0	-4.63	-4.04	-0.59	-0.0314	0.0285	0.05	-3.99	-0.64
3-methylpyridine	0	-4.77	-4.45	-0.32	-0.0320	0.0281	-0.11	-4.57	-0.20
4-methylpyridine	0	-4.94	-4.57	-0.37	-0.0322	0.0270	-0.18	-4.74	-0.20
4-ethylpyridine	0	-4.74	-4.56	-0.18	-0.0323	0.0270	-0.18	-4.74	0.00
2,4-dimethylpyridine	0	-4.86	-4.18	-0.68	-0.0321	0.0259	-0.13	-4.30	-0.56

2,5-dimethylpyridine	0	-4.72	-4.06	-0.66	-0.0317	0.0271	-0.04	-4.10	-0.62
2,6-dimethylpyridine	0	-4.60	-3.70	-0.90	-0.0312	0.0277	0.10	-3.60	-1.00
3,4-dimethylpyridine	0	-5.22	-4.71	-0.51	-0.0326	0.0264	-0.29	-5.00	-0.22
3,5-dimethylpyridine	0	-4.84	-4.48	-0.36	-0.0325	0.0268	-0.23	-4.72	-0.12
aniline	0	-5.49	-6.49	1.00	-0.0257	0.0536	0.95	-5.54	0.05
N-methylaniline	0	-4.68	-5.10	0.42	-0.0221	0.0528	1.42	-3.68	-1.00
2-methylaniline	0	-5.56	-5.95	0.39	-0.0260	0.0518	0.93	-5.02	-0.54
3-methylaniline	0	-5.67	-6.34	0.67	-0.0260	0.0525	0.91	-5.42	-0.25
4-methylaniline	0	-5.55	-6.27	0.72	-0.0263	0.0513	0.90	-5.38	-0.17
N-ethylaniline	0	-4.62	-4.96	0.34	-0.0195	0.0533	1.65	-3.31	-1.31
3-aminoaniline	0	-9.92	-10.42	0.50	-0.0262	0.0523	0.89	-9.53	-0.39
N,N-dimethylaniline	0	-3.58	-3.78	0.20	-0.0176	0.0237	2.05	-1.74	-1.84
piperazine	0	-7.40	-4.93	-2.47	-0.0310	0.0414	0.06	-4.88	-2.52
N-methylpiperazine	0	-7.77	-3.91	-3.86	-0.0308	0.0418	0.10	-3.81	-3.96
N,N'-dimethylpiperazine	0	-7.58	-2.86	-4.72	-0.0287	0.0187	0.69	-2.17	-5.41
1-methylthymine	0	-10.40	-12.54	2.14	-0.0307	0.0730	-0.65	-13.18	2.78
9-methyladenine	0	-13.60	-11.13	-2.47	-0.0308	0.0649	-0.36	-11.48	-2.12
acetamide	0	-9.71	-9.91	0.20	-0.0323	0.0650	-0.76	-10.67	0.96
E-N-methylacetamide	0	-10.00	-8.80	-1.20	-0.0337	0.0589	-0.99	-9.78	-0.22
Z-N-methylacetamide	0	-10.00	-8.39	-1.61	-0.0339	0.0642	-1.21	-9.59	-0.41
benzamide	0	-10.90	-9.93	-0.97	-0.0314	0.0638	-0.48	-10.41	-0.49
2,6-dichlorothiobenzamide	0	-10.81	-11.58	0.77	-0.0197	0.0766	0.86	-10.72	-0.09
urea	0	-13.80	-12.65	-1.15	-0.0316	0.0629	-0.50	-13.15	-0.65
1,1-dimethyl-3-phenylurea	0	-9.63	-9.45	-0.18	-0.0306	0.0578	-0.12	-9.57	-0.06
hydrazine	0	-6.26	-7.38	1.12	-0.0318	0.0436	-0.17	-7.55	1.29
methylhydrazine	0	-5.31	-6.55	1.24	-0.0317	0.0442	-0.14	-6.69	1.38
1,1-dimethylhydrazine	0	-4.48	-5.05	0.57	-0.0316	0.0445	-0.13	-5.18	0.70
2-methylpyrazine	0	-5.57	-4.81	-0.76	-0.0282	0.0290	0.77	-4.04	-1.53
2-ethylpyrazine	0	-5.51	-4.45	-1.06	-0.0283	0.0289	0.75	-3.70	-1.81
morpholine	0	-7.17	-5.09	-2.08	-0.0297	0.0438	0.34	-4.76	-2.41
N-methylmorpholine	0	-6.34	-3.94	-2.40	-0.0286	0.0213	0.72	-3.22	-3.12
acetonitrile	0	-3.89	-6.74	2.85	-0.0271	0.0364	0.93	-5.81	1.92
butanonitrile	0	-3.64	-6.15	2.51	-0.0272	0.0331	0.94	-5.20	1.56
propionitrile	0	-3.85	-6.37	2.52	-0.0273	0.0332	0.93	-5.44	1.59
benzonitrile	0	-4.10	-6.52	2.42	-0.0267	0.0332	1.03	-5.49	1.39

2,6-dichlorobenzonitrile	0	-5.22	-6.87	1.65	-0.0255	0.0366	1.20	-5.67	0.45
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-8.98	-0.02	-0.0254	0.0705	0.50	-8.48	-0.52
trimethylphosphate	0	-8.70	-8.88	0.18	-0.0303	0.0308	0.32	-8.56	-0.14
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-8.14	1.53	-0.0267	0.0411	0.97	-7.17	0.56
phosphine	0	0.60	-0.97	1.57	-0.0127	0.0227	2.25	1.28	-0.68
hydrogen sulfide	0	-0.70	-3.02	2.32	-0.0141	0.0332	2.17	-0.85	0.15
dimethyl sulfide	0	-1.54	-2.88	1.34	-0.0177	0.0258	2.04	-0.84	-0.70
diethyl sulfide	0	-1.43	-2.63	1.20	-0.0182	0.0210	2.02	-0.61	-0.82
dipropyl sulfide	0	-1.27	-2.72	1.45	-0.0183	0.0205	2.01	-0.71	-0.56
bis(2-chloroethyl)sulfide	0	-3.92	-5.83	1.91	-0.0131	0.0310	2.21	-3.62	-0.30
dimethyl disulfide	0	-1.83	-3.45	1.62	-0.0139	0.0284	2.20	-1.26	-0.57
diethyl disulfide	0	-1.63	-3.02	1.39	-0.0143	0.0257	2.19	-0.83	-0.80
methanethiol	0	-1.24	-2.95	1.71	-0.0163	0.0282	2.10	-0.85	-0.39
ethanethiol	0	-1.30	-2.83	1.53	-0.0164	0.0272	2.10	-0.73	-0.57
1-propanethiol	0	-1.05	-2.86	1.81	-0.0163	0.0271	2.10	-0.76	-0.29
thiophene	0	-1.42	-2.87	1.45	-0.0073	0.0330	2.28	-0.58	-0.84
thiophenol	0	-2.55	-4.12	1.57	-0.0121	0.0329	2.22	-1.90	-0.65
thioanisole	0	-2.73	-4.11	1.38	-0.0135	0.0293	2.20	-1.91	-0.82
tetramethylsilane	0	3.04	-0.97	4.01	-0.0030	0.0180	2.34	1.37	1.67
acetylene	-1	-76.50	-65.51	-10.99	-0.0531	0.0132	-12.68	-78.19	1.69
acetonitrile	-1	-66.60	-59.82	-6.78	-0.0503	0.0020	-10.03	-69.86	3.26
cyanamide	-1	-72.20	-64.23	-7.97	-0.0508	0.0214	-10.47	-74.70	2.50
aniline	-1	-62.90	-54.81	-8.09	-0.0538	0.0079	-13.39	-68.20	5.30
diphenylamine	-1	-54.60	-47.44	-7.16	-0.0465	0.0117	-6.97	-54.41	-0.19
hydrogen cyanide	-1	-70.20	-65.61	-4.59	-0.0497	-0.0346	-9.52	-75.13	4.93
formic acid	-1	-76.20	-64.96	-11.24	-0.0511	-0.0063	-10.76	-75.73	-0.47
acetic acid	-1	-77.60	-64.17	-13.43	-0.0524	0.0075	-12.02	-76.19	-1.41
propanoic acid	-1	-76.20	-62.19	-14.01	-0.0525	0.0078	-12.06	-74.25	-1.95
hexanoic acid	-1	-74.60	-61.30	-13.30	-0.0524	0.0144	-12.04	-73.34	-1.26
acrylic acid	-1	-74.00	-62.72	-11.28	-0.0520	0.0151	-11.64	-74.36	0.36
pyruvic acid	-1	-68.50	-61.75	-6.75	-0.0496	0.0180	-9.42	-71.17	2.67
benzoic acid	-1	-71.20	-59.92	-11.28	-0.0514	0.0183	-11.02	-70.94	-0.26
methanol	-1	-95.00	-67.60	-27.40	-0.0619	-0.0156	-23.80	-91.40	-3.60
ethanol	-1	-90.70	-63.85	-26.85	-0.0618	0.0004	-23.63	-87.49	-3.21
1-propanol	-1	-88.30	-63.17	-25.13	-0.0619	0.0073	-23.81	-86.98	-1.32

isopropanol	-1	-86.30	-60.88	-25.42	-0.0610	0.0009	-22.51	-83.39	-2.91
2-butanol	-1	-84.20	-58.08	-26.12	-0.0605	0.0017	-21.66	-79.74	-4.46
t-butanol	-1	-82.30	-58.58	-23.72	-0.0603	0.0016	-21.40	-79.98	-2.32
allyl alcohol	-1	-86.60	-62.69	-23.91	-0.0610	0.0090	-22.47	-85.16	-1.44
benzyl alcohol	-1	-85.10	-58.48	-26.62	-0.0599	0.0147	-20.92	-79.41	-5.69
2-methoxyethanol	-1	-89.40	-64.62	-24.78	-0.0616	0.0132	-23.26	-87.88	-1.52
phenol	-1	-71.90	-56.55	-15.35	-0.0540	0.0088	-13.62	-70.17	-1.73
2-methylphenol	-1	-70.20	-54.73	-15.47	-0.0540	0.0078	-13.61	-68.34	-1.86
3-methylphenol	-1	-71.10	-56.31	-14.79	-0.0543	0.0122	-13.95	-70.26	-0.84
4-methylphenol	-1	-72.00	-56.31	-15.69	-0.0546	0.0110	-14.30	-70.61	-1.39
1,2-ethanediol	-1	-85.30	-68.14	-17.16	-0.0618	0.0580	-23.96	-92.10	6.80
3-hydroxyphenol	-1	-73.80	-58.71	-15.09	-0.0533	0.0648	-13.48	-72.19	-1.61
4-hydroxyphenol	-1	-77.60	-60.23	-17.37	-0.0547	0.0632	-14.96	-75.19	-2.41
methyl hydroperoxide	-1	-93.20	-69.73	-23.47	-0.0608	0.0030	-22.12	-91.85	-1.35
ethyl hydroperoxide	-1	-89.20	-68.92	-20.28	-0.0610	0.0110	-22.40	-91.31	2.11
acetaldehyde	-1	-76.50	-61.67	-14.83	-0.0555	-0.0006	-15.25	-76.92	0.42
acetone	-1	-76.20	-60.10	-16.10	-0.0557	0.0046	-15.52	-75.61	-0.59
3-pentanone	-1	-73.70	-55.29	-18.41	-0.0546	0.0069	-14.27	-69.56	-4.14
water	-1	-104.70	-77.94	-26.76	-0.0660	0.0023	-30.50	-108.44	3.74
hydrogen peroxide	-1	-97.30	-75.73	-21.57	-0.0613	0.0396	-22.93	-98.66	1.36
hydroperoxyl radical	-1	-83.30	-71.74	-11.56	-0.0536	-0.0420	-13.21	-84.96	1.66
2-nitrophenol	-1	-60.10	-54.48	-5.62	-0.0477	0.0170	-7.87	-62.35	2.25
3-nitrophenol	-1	-61.90	-51.26	-10.64	-0.0503	0.0211	-10.06	-61.32	-0.58
4-nitrophenol	-1	-57.80	-49.73	-8.07	-0.0459	0.0182	-6.59	-56.32	-1.48
nitromethane	-1	-76.50	-62.63	-13.87	-0.0501	0.0102	-9.87	-72.50	-4.00
4-nitroaniline	-1	-57.40	-49.89	-7.51	-0.0453	0.0200	-6.18	-56.07	-1.33
acetamide	-1	-80.20	-61.86	-18.34	-0.0527	0.0057	-12.26	-74.12	-6.08
methanethiol	-1	-73.80	-61.52	-12.28	-0.0432	0.0027	-4.80	-66.31	-7.49
ethanethiol	-1	-71.80	-59.09	-12.71	-0.0427	0.0056	-4.51	-63.60	-8.20
1-propanethiol	-1	-70.50	-58.86	-11.64	-0.0428	0.0108	-4.55	-63.41	-7.09
thiophenol	-1	-63.40	-54.08	-9.32	-0.0386	0.0142	-2.44	-56.52	-6.88
hydrogen sulfide	-1	-72.10	-62.96	-9.14	-0.0428	-0.0059	-4.57	-67.52	-4.58
dimethyl sulfoxide	-1	-67.70	-58.29	-9.41	-0.0533	0.0114	-12.92	-71.21	3.51
hydrofluoric acid	-1	-104.40	-83.15	-21.25	-0.0682	-0.0682	-34.63	-117.77	13.37
hydrochloric acid	-1	-74.50	-66.84	-7.66	-0.0426	-0.0426	-4.46	-71.30	-3.20

hydrobromic acid	-1	-68.30	-62.85	-5.45	-0.0372	-0.0372	-1.82	-64.67	-3.63
chloroform	-1	-54.10	-50.41	-3.69	-0.0387	-0.0055	-2.47	-52.88	-1.22
trifluoroacetic acid	-1	-59.30	-57.35	-1.95	-0.0464	0.0264	-6.94	-64.29	4.99
chloroacetic acid	-1	-69.70	-59.30	-10.40	-0.0486	0.0171	-8.60	-67.90	-1.80
dichloroacetic acid	-1	-62.30	-55.85	-6.45	-0.0461	0.0236	-6.71	-62.56	0.26
2,2,2-trifluoroethanol	-1	-77.50	-60.07	-17.43	-0.0582	0.0086	-18.56	-78.64	1.14
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-55.06	-10.44	-0.0542	0.0147	-13.89	-68.96	3.46
2-chlorophenol	-1	-66.10	-54.20	-11.90	-0.0519	0.0142	-11.53	-65.73	-0.37
4-chlorophenol	-1	-66.00	-52.70	-13.30	-0.0524	0.0141	-12.04	-64.74	-1.26
methylamine	1	-76.40	-75.81	-0.59	0.0269	0.1055	-1.03	-76.83	0.43
n-propylamine	1	-71.50	-70.68	-0.82	0.0073	0.1047	-0.93	-71.61	0.11
isopropylamine	1	-69.60	-68.88	-0.72	0.0109	0.1023	-0.67	-69.55	-0.05
tert-butylamine	1	-67.30	-66.08	-1.22	0.0109	0.1005	-0.49	-66.57	-0.73
cyclohexanamine	1	-68.70	-65.74	-2.96	0.0079	0.1011	-0.55	-66.29	-2.41
allylamine	1	-72.00	-70.91	-1.09	-0.0063	0.1056	-1.05	-71.96	-0.04
dimethylamine	1	-68.60	-67.93	-0.67	0.0249	0.1004	-0.48	-68.41	-0.19
diethylamine	1	-63.40	-61.60	-1.80	0.0115	0.0940	0.12	-61.49	-1.91
di-n-propylamine	1	-60.50	-59.35	-1.15	0.0079	0.0939	0.13	-59.22	-1.28
diallylamine	1	-61.60	-60.08	-1.52	-0.0033	0.0960	-0.06	-60.14	-1.46
trimethylamine	1	-61.10	-61.10	0.00	0.0241	0.0963	-0.08	-61.19	0.09
triethylamine	1	-54.60	-53.13	-1.47	0.0098	0.0830	0.92	-52.21	-2.39
aniline	1	-72.40	-70.13	-2.27	0.0034	0.1089	-1.44	-71.56	-0.84
2-methylaniline	1	-70.30	-67.76	-2.54	0.0024	0.1063	-1.13	-68.89	-1.41
3-methylaniline	1	-69.60	-68.45	-1.15	0.0021	0.1082	-1.35	-69.80	0.20
4-methylaniline	1	-69.80	-68.28	-1.52	0.0032	0.1078	-1.30	-69.58	-0.22
3-aminoaniline	1	-65.80	-70.62	4.82	-0.0145	0.1069	-1.33	-71.95	6.15
N-methylaniline	1	-62.60	-62.32	-0.28	0.0031	0.1016	-0.60	-62.93	0.33
N-ethylaniline	1	-62.20	-59.39	-2.81	0.0030	0.0982	-0.26	-59.65	-2.55
N,N-dimethylaniline	1	-57.20	-55.74	-1.46	0.0031	0.0941	0.11	-55.63	-1.57
4-methyl-N,N-dimethylaniline	1	-55.90	-54.24	-1.66	0.0029	0.0930	0.20	-54.04	-1.86
N,N-diethylaniline	1	-54.00	-51.30	-2.70	0.0023	0.0866	0.69	-50.61	-3.39
1-aminonaphthalene	1	-67.40	-66.54	-0.86	0.0009	0.1099	-1.56	-68.10	0.70
aziridine	1	-70.90	-69.90	-1.00	0.0254	0.1068	-1.18	-71.08	0.18
azetidine	1	-67.70	-65.91	-1.79	0.0176	0.1000	-0.43	-66.34	-1.36
pyrrolidine	1	-66.00	-63.57	-2.43	0.0125	0.0988	-0.32	-63.89	-2.11

piperidine	1	-64.20	-61.63	-2.57	0.0138	0.0991	-0.35	-61.99	-2.21
azacycloheptane	1	-63.30	-59.98	-3.32	0.0089	0.0991	-0.34	-60.32	-2.98
pyrrole	1	-61.40	-61.69	0.29	0.0143	0.1042	-0.88	-62.57	1.17
pyridine	1	-61.10	-60.07	-1.03	0.0178	0.1063	-1.12	-61.18	0.08
quinoline	1	-56.00	-54.03	-1.97	0.0068	0.0995	-0.38	-54.42	-1.58
piperazine	1	-66.00	-63.98	-2.02	-0.0200	0.0999	-0.87	-64.85	-1.15
acetonitrile	1	-75.30	-69.86	-5.44	0.0327	0.1405	-7.12	-76.99	1.69
ammonia	1	-85.20	-85.50	0.30	0.0569	0.1120	-1.84	-87.34	2.14
hydrazine	1	-84.60	-84.16	-0.44	-0.0095	0.1105	-1.66	-85.83	1.23
methanol	1	-93.00	-82.98	-10.02	0.0143	0.1511	-9.96	-92.94	-0.06
ethanol	1	-88.40	-77.25	-11.15	0.0093	0.1488	-9.29	-86.54	-1.86
dimethyl ether	1	-79.70	-69.78	-9.92	0.0113	0.1432	-7.79	-77.57	-2.13
diethyl ether	1	-71.50	-61.40	-10.10	0.0071	0.1291	-4.64	-66.04	-5.46
acetone	1	-77.10	-66.81	-10.29	0.0064	0.1300	-4.82	-71.63	-5.47
acetophenone	1	-64.50	-55.24	-9.26	0.0023	0.1092	-1.47	-56.71	-7.79
water	1	-110.30	-100.52	-9.78	0.0186	0.1634	-13.94	-114.45	4.15
4-methoxyaniline	1	-71.20	-68.86	-2.34	-0.0174	0.1075	-1.54	-70.40	-0.80
4-nitroaniline	1	-75.90	-82.03	6.13	-0.0155	0.1136	-2.24	-84.27	8.37
morpholine	1	-69.60	-67.96	-1.64	-0.0159	0.1029	-0.93	-68.89	-0.71
acetamide	1	-73.90	-72.69	-1.21	0.0006	0.1238	-3.66	-76.35	2.45
benzamide	1	-67.20	-64.41	-2.79	-0.0001	0.1208	-3.14	-67.55	0.35
dimethyl sulfide	1	-64.50	-62.98	-1.52	0.0201	0.0698	1.58	-61.40	-3.10
dimethyl sulfoxide	1	-67.70	-64.78	-2.92	-0.0033	0.1191	-2.88	-67.66	-0.04
3-chloroaniline	1	-74.70	-72.88	-1.82	-0.0031	0.1104	-1.63	-74.51	-0.19
4-chloroaniline	1	-74.10	-73.07	-1.03	-0.0016	0.1111	-1.71	-74.79	0.69
PEARSON			0.99					1.00	

Table S 4-3

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/6-31+G* method for the cavity surface with constant density = 0.002 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.50	2.50	0.0047	0.0330	4.16	3.65	-1.65
ethane	0	1.83	-0.48	2.31	0.0044	0.0294	4.16	3.68	-1.85
n-propane	0	1.96	-0.58	2.54	0.0044	0.0292	4.16	3.58	-1.62
n-butane	0	2.08	-0.67	2.75	0.0045	0.0292	4.16	3.49	-1.41
n-pentane	0	2.33	-0.75	3.08	0.0042	0.0290	4.16	3.41	-1.08
n-hexane	0	2.49	-0.83	3.32	0.0044	0.0291	4.16	3.33	-0.84
n-heptane	0	2.62	-0.91	3.53	0.0047	0.0284	4.16	3.25	-0.63
n-octane	0	2.89	-0.97	3.86	0.0042	0.0282	4.16	3.18	-0.29
2-methylpropane	0	2.32	-0.75	3.07	0.0045	0.0292	4.16	3.41	-1.09
2,2-dimethylpropane	0	2.50	-0.94	3.44	0.0046	0.0293	4.16	3.22	-0.72
2-methylpentane	0	2.52	-0.88	3.40	0.0032	0.0291	4.16	3.28	-0.76
2,4-dimethylpentane	0	2.88	-1.05	3.93	0.0037	0.0296	4.16	3.11	-0.23
2,2,4-trimethylpentane	0	2.85	-1.21	4.06	0.0014	0.0294	4.16	2.94	-0.09
cyclopropane	0	0.75	-1.82	2.57	-0.0091	0.0356	4.15	2.33	-1.58
cyclopentane	0	1.20	-0.64	1.84	0.0045	0.0284	4.16	3.51	-2.31
cyclohexane	0	1.23	-0.58	1.81	0.0047	0.0269	4.16	3.58	-2.35
methylcyclohexane	0	1.71	-0.73	2.44	0.0042	0.0287	4.16	3.43	-1.72
cis-1,2-dimethylcyclohexane	0	1.58	-0.86	2.44	0.0026	0.0292	4.16	3.30	-1.72
ethene	0	1.27	-1.95	3.22	-0.0101	0.0398	4.14	2.20	-0.93
propene	0	1.27	-1.93	3.20	-0.0114	0.0371	4.14	2.21	-0.94
1-butene	0	1.38	-1.93	3.31	-0.0117	0.0362	4.13	2.21	-0.83
1-pentene	0	1.66	-2.01	3.67	-0.0115	0.0359	4.14	2.12	-0.46
E-2-pentene	0	1.34	-1.77	3.11	-0.0117	0.0337	4.13	2.36	-1.02
1-hexene	0	1.68	-2.16	3.84	-0.0108	0.0367	4.14	1.98	-0.30
2-methylpropene	0	1.16	-2.03	3.19	-0.0121	0.0347	4.13	2.10	-0.94
s-trans-1,3-butadiene	0	0.61	-3.07	3.68	-0.0073	0.0403	4.15	1.09	-0.48
cyclopentene	0	0.56	-1.60	2.16	-0.0120	0.0372	4.13	2.54	-1.98
ethyne	0	-0.01	-5.20	5.19	-0.0098	0.0738	4.16	-1.04	1.03
propyne	0	-0.31	-4.49	4.18	-0.0130	0.0693	4.13	-0.36	0.05
1-butyne	0	-0.16	-4.36	4.20	-0.0131	0.0693	4.13	-0.23	0.07
1-pentyne	0	0.01	-4.26	4.27	-0.0142	0.0691	4.12	-0.14	0.15
1-hexyne	0	0.29	-4.57	4.86	-0.0132	0.0688	4.13	-0.44	0.73

butenyne	0	0.04	-4.82	4.86	-0.0113	0.0727	4.15	-0.67	0.71
benzene	0	-0.87	-3.56	2.69	-0.0009	0.0402	4.16	0.60	-1.47
ethylbenzene	0	-0.80	-3.58	2.78	-0.0023	0.0393	4.16	0.58	-1.38
naphthalene	0	-2.39	-4.92	2.53	-0.0020	0.0407	4.16	-0.76	-1.63
anthracene	0	-4.23	-6.26	2.03	-0.0023	0.0410	4.16	-2.10	-2.13
toluene	0	-0.89	-3.52	2.63	-0.0022	0.0393	4.16	0.64	-1.53
p-xylene	0	-0.81	-3.44	2.63	-0.0037	0.0371	4.16	0.72	-1.53
m-xylene	0	-0.84	-3.47	2.63	-0.0037	0.0385	4.16	0.69	-1.53
o-xylene	0	-0.90	-3.59	2.69	-0.0033	0.0383	4.16	0.56	-1.46
fluoromethane	0	-0.22	-3.93	3.71	-0.0200	0.0413	3.98	0.05	-0.27
chloromethane	0	-0.56	-3.75	3.19	-0.0079	0.0479	4.15	0.40	-0.96
bromomethane	0	-0.82	-3.69	2.87	-0.0051	0.0489	4.16	0.47	-1.29
chlorofluoromethane	0	-0.77	-5.50	4.73	-0.0111	0.0574	4.14	-1.36	0.59
dichloromethane	0	-1.36	-5.25	3.89	-0.0026	0.0614	4.16	-1.09	-0.27
dibromomethane	0	-2.11	-5.34	3.23	-0.0005	0.0616	4.16	-1.18	-0.93
chlorodifluoromethane	0	-0.50	-5.00	4.50	-0.0039	0.0689	4.17	-0.83	0.33
chloroform	0	-1.07	-4.69	3.62	0.0022	0.0726	4.17	-0.52	-0.55
chloroethane	0	-0.63	-3.73	3.10	-0.0089	0.0452	4.15	0.42	-1.05
bromoethane	0	-0.70	-3.67	2.97	-0.0061	0.0462	4.16	0.49	-1.19
bromoform	0	-1.98	-5.37	3.39	0.0034	0.0716	4.17	-1.20	-0.78
tetrafluoromethane	0	3.16	-1.87	5.03	0.0026	0.0713	4.17	2.30	0.86
difluorodichloromethane	0	1.69	-1.86	3.55	0.0021	0.0528	4.16	2.30	-0.61
fluorotrichloromethane	0	0.82	-2.07	2.89	0.0014	0.0495	4.16	2.09	-1.27
bromotrifluoromethane	0	1.79	-2.24	4.03	0.0021	0.0706	4.17	1.93	-0.14
bromotrichloromethane	0	-0.93	-2.83	1.90	0.0053	0.0620	4.16	1.34	-2.27
hexafluoroethane	0	3.94	-2.02	5.96	0.0026	0.0705	4.17	2.15	1.79
hexachloroethane	0	-1.40	-3.10	1.70	0.0047	0.0483	4.16	1.06	-2.46
chloropentafluoroethane	0	2.86	-2.00	4.86	0.0017	0.0668	4.17	2.17	0.69
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-2.30	4.07	-0.0002	0.0503	4.16	1.86	-0.09
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-5.67	6.19	-0.0056	0.0717	4.17	-1.50	2.02
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-5.44	5.31	-0.0019	0.0735	4.17	-1.27	1.14
1-chloro-2,2,2-trifluoroethane	0	0.06	-5.83	5.89	-0.0039	0.0624	4.16	-1.66	1.72
1,1,1,2-tetrachloroethane	0	-1.15	-5.42	4.27	-0.0023	0.0613	4.16	-1.26	0.11
1,1,1-trichloroethane	0	-0.25	-3.70	3.45	-0.0001	0.0484	4.16	0.46	-0.71
1,1,2-trichloroethane	0	-1.95	-6.54	4.59	-0.0042	0.0640	4.16	-2.38	0.43

1,1-difluoroethane	0	-0.11	-5.20	5.09	-0.0139	0.0497	4.11	-1.09	0.98
1-bromo-2-chloroethane	0	-1.95	-5.53	3.58	-0.0055	0.0519	4.16	-1.37	-0.58
octafluoropropane	0	4.28	-2.32	6.60	0.0027	0.0683	4.17	1.84	2.44
2-chloropropane	0	-0.25	-3.74	3.49	-0.0096	0.0431	4.15	0.40	-0.65
1-chloropropane	0	-0.27	-3.74	3.47	-0.0089	0.0443	4.15	0.41	-0.68
1-bromopropane	0	-0.56	-3.70	3.14	-0.0061	0.0453	4.16	0.46	-1.02
2-bromopropane	0	-0.48	-3.66	3.18	-0.0069	0.0444	4.16	0.49	-0.97
2-chlorobutane	0	0.07	-3.59	3.66	-0.0097	0.0423	4.15	0.56	-0.49
1-bromobutane	0	-0.41	-3.76	3.35	-0.0062	0.0452	4.16	0.39	-0.80
1-chloropentane	0	0.07	-3.93	4.00	-0.0089	0.0443	4.15	0.22	-0.15
2-chloropentane	0	0.07	-3.63	3.70	-0.0097	0.0421	4.15	0.52	-0.45
1-bromopentane	0	-0.08	-3.86	3.78	-0.0062	0.0453	4.16	0.29	-0.37
1-bromo-isobutane	0	-0.03	-3.60	3.57	-0.0062	0.0454	4.16	0.56	-0.59
tetrachloroethene	0	0.05	-2.44	2.49	0.0042	0.0466	4.16	1.72	-1.67
trichloroethene	0	-0.39	-3.34	2.95	0.0020	0.0654	4.17	0.82	-1.21
chloroethene	0	-0.59	-3.31	2.72	-0.0044	0.0542	4.16	0.86	-1.45
E-1,2-dichloroethene	0	-0.76	-3.73	2.97	-0.0013	0.0602	4.16	0.43	-1.19
Z-1,2-dichloroethene	0	-1.17	-4.45	3.28	-0.0008	0.0614	4.16	-0.29	-0.88
3-chloropropene	0	-0.57	-4.58	4.01	-0.0081	0.0490	4.15	-0.42	-0.15
3-bromopropene	0	-0.86	-4.87	4.01	-0.0059	0.0498	4.16	-0.72	-0.14
fluorobenzene	0	-0.78	-4.30	3.52	-0.0139	0.0467	4.11	-0.18	-0.60
chlorobenzene	0	-1.12	-4.07	2.95	-0.0040	0.0464	4.16	0.09	-1.21
bromobenzene	0	-1.46	-4.20	2.74	-0.0021	0.0464	4.16	-0.04	-1.42
1,4-dichlorobenzene	0	-1.01	-4.47	3.46	-0.0027	0.0506	4.16	-0.31	-0.70
1,2-dichlorobenzene	0	-1.36	-4.49	3.13	-0.0031	0.0500	4.16	-0.33	-1.03
p-dibromobenzene	0	-2.30	-4.73	2.43	-0.0006	0.0501	4.16	-0.57	-1.73
chlorotoluene	0	-1.92	-6.48	4.56	-0.0088	0.0479	4.15	-2.32	0.40
o-chlorotoluene	0	-1.15	-3.84	2.69	-0.0051	0.0459	4.16	0.32	-1.47
bromotoluene	0	-2.37	-6.46	4.09	-0.0062	0.0493	4.16	-2.30	-0.07
p-bromotoluene	0	-1.39	-4.18	2.79	-0.0026	0.0457	4.16	-0.02	-1.37
2,3-dichlorobiphenyl	0	-2.45	-6.41	3.96	-0.0032	0.0494	4.16	-2.25	-0.20
2,2'-dichlorobiphenyl	0	-2.73	-6.92	4.19	-0.0049	0.0465	4.16	-2.76	0.03
2,2',3'-trichlorobiphenyl	0	-1.99	-6.94	4.95	-0.0062	0.0498	4.16	-2.79	0.80
1,2-dimethoxyethane	0	-4.84	-6.43	1.59	-0.0316	0.0364	3.12	-3.31	-1.53
anisole	0	-2.45	-5.88	3.43	-0.0268	0.0423	3.60	-2.27	-0.18

dimethyl ether	0	-1.92	-4.17	2.25	-0.0330	0.0366	2.93	-1.24	-0.68
diethyl ether	0	-1.76	-4.31	2.55	-0.0339	0.0337	2.79	-1.52	-0.24
isopropyl ether	0	-0.53	-4.26	3.73	-0.0340	0.0337	2.78	-1.49	0.96
methyl propyl ether	0	-1.66	-4.03	2.37	-0.0328	0.0358	2.96	-1.07	-0.59
methyl isopropyl ether	0	-2.01	-4.08	2.07	-0.0332	0.0352	2.90	-1.18	-0.83
t-butyl methyl ether	0	-2.21	-4.14	1.93	-0.0335	0.0345	2.87	-1.28	-0.93
ethyl phenyl ether	0	-2.22	-5.71	3.49	-0.0269	0.0421	3.60	-2.11	-0.11
tetrahydrofuran	0	-3.47	-4.60	1.13	-0.0346	0.0352	2.69	-1.91	-1.56
tetrahydropyran	0	-3.12	-4.21	1.09	-0.0342	0.0333	2.76	-1.46	-1.66
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-7.05	6.93	-0.0188	0.0597	4.02	-3.03	2.91
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-8.45	8.56	-0.0118	0.0724	4.15	-4.31	4.42
acetaldehyde	0	-3.50	-7.06	3.56	-0.0319	0.0463	3.08	-3.98	0.48
propanal	0	-3.44	-6.70	3.26	-0.0320	0.0442	3.07	-3.63	0.19
butanal	0	-3.18	-6.94	3.76	-0.0321	0.0443	3.06	-3.88	0.70
pentanal	0	-3.03	-6.84	3.81	-0.0323	0.0435	3.03	-3.81	0.78
octanal	0	-2.29	-6.85	4.56	-0.0317	0.0412	3.10	-3.75	1.46
benzaldehyde	0	-4.02	-8.15	4.13	-0.0330	0.0472	2.93	-5.22	1.20
p-hydroxybenzaldehyde	0	-10.48	-15.39	4.91	-0.0344	0.1217	2.81	-12.58	2.10
m-hydroxybenzaldehyde	0	-9.51	-14.79	5.28	-0.0326	0.1206	3.07	-11.72	2.21
acetone	0	-3.85	-7.61	3.76	-0.0339	0.0441	2.80	-4.81	0.96
2-butanone	0	-3.64	-7.20	3.56	-0.0343	0.0436	2.74	-4.46	0.82
2-pentanone	0	-3.53	-7.25	3.72	-0.0341	0.0434	2.77	-4.48	0.95
3-pentanone	0	-3.41	-6.80	3.39	-0.0326	0.0408	2.99	-3.81	0.40
2-hexanone	0	-3.29	-7.35	4.06	-0.0341	0.0431	2.77	-4.58	1.29
2-heptanone	0	-3.04	-7.35	4.31	-0.0340	0.0431	2.79	-4.56	1.52
4-heptanone	0	-2.93	-6.91	3.98	-0.0328	0.0406	2.96	-3.96	1.03
2-octanone	0	-2.88	-7.36	4.48	-0.0339	0.0427	2.80	-4.56	1.68
5-nonanone	0	-2.67	-7.02	4.35	-0.0328	0.0404	2.96	-4.06	1.39
3,3-dimethylbutanone	0	-2.89	-6.98	4.09	-0.0344	0.0444	2.73	-4.25	1.36
cyclopentanone	0	-4.68	-7.51	2.83	-0.0338	0.0420	2.82	-4.69	0.01
acetophenone	0	-4.58	-8.48	3.90	-0.0345	0.0449	2.71	-5.77	1.19
methyl formate	0	-2.78	-7.60	4.82	-0.0293	0.0545	3.38	-4.21	1.43
ethyl formate	0	-2.65	-7.51	4.86	-0.0298	0.0534	3.33	-4.19	1.54
methyl acetate	0	-3.32	-7.56	4.24	-0.0317	0.0459	3.10	-4.46	1.14
ethyl acetate	0	-3.10	-7.54	4.44	-0.0322	0.0448	3.05	-4.49	1.39

propyl acetate	0	-2.86	-7.56	4.70	-0.0323	0.0453	3.03	-4.54	1.68
butyl acetate	0	-2.55	-7.59	5.04	-0.0321	0.0441	3.06	-4.53	1.98
methyl propanoate	0	-2.93	-7.28	4.35	-0.0311	0.0450	3.18	-4.09	1.16
methyl butanoate	0	-2.83	-7.33	4.50	-0.0313	0.0447	3.15	-4.18	1.35
methyl pentanoate	0	-2.57	-7.40	4.83	-0.0310	0.0445	3.19	-4.21	1.64
methyl hexanoate	0	-2.49	-7.46	4.97	-0.0314	0.0444	3.15	-4.31	1.82
methyl benzoate	0	-3.91	-8.10	4.19	-0.0318	0.0453	3.09	-5.01	1.10
hydrogen	0	2.33	-0.21	2.54	0.0063	0.0291	4.16	3.95	-1.62
water	0	-6.31	-11.93	5.62	-0.0345	0.1066	2.75	-9.17	2.86
water dimer	0	-11.27	-18.88	7.61	-0.0391	0.1149	1.90	-16.98	5.71
hydrogen peroxide	0	-8.58	-13.22	4.64	-0.0272	0.1164	3.64	-9.57	0.99
methyl peroxide	0	-5.28	-9.68	4.40	-0.0280	0.1153	3.58	-6.10	0.82
ethyl peroxide	0	-5.32	-9.65	4.33	-0.0283	0.1135	3.54	-6.10	0.78
1,4-dioxane	0	-5.05	-7.35	2.30	-0.0320	0.0392	3.07	-4.28	-0.77
methanol	0	-5.11	-8.09	2.98	-0.0342	0.1029	2.80	-5.29	0.18
ethanol	0	-5.01	-7.75	2.74	-0.0340	0.1024	2.83	-4.92	-0.09
1-propanol	0	-4.83	-7.77	2.94	-0.0339	0.1017	2.84	-4.93	0.10
isopropanol	0	-4.76	-7.63	2.87	-0.0347	0.0975	2.72	-4.91	0.15
1-butanol	0	-4.72	-7.85	3.13	-0.0339	0.1015	2.85	-5.01	0.29
t-butanol	0	-4.51	-7.45	2.94	-0.0343	0.0968	2.78	-4.67	0.16
1-pentanol	0	-4.47	-8.00	3.53	-0.0345	0.0988	2.75	-5.25	0.78
1-hexanol	0	-4.36	-8.32	3.96	-0.0347	0.1015	2.71	-5.61	1.25
1-heptanol	0	-4.24	-7.91	3.67	-0.0346	0.0972	2.72	-5.19	0.95
1-octanol	0	-4.09	-5.63	1.54	-0.0298	0.0669	3.34	-2.29	-1.80
allyl alcohol	0	-5.08	-8.31	3.23	-0.0335	0.1018	2.91	-5.40	0.32
cyclopentanol	0	-5.49	-7.28	1.79	-0.0346	0.0940	2.72	-4.56	-0.93
2-methoxyethanol	0	-6.77	-10.84	4.07	-0.0328	0.1052	3.01	-7.83	1.06
2,2,2-trifluoroethanol	0	-4.31	-11.74	7.43	-0.0259	0.1165	3.74	-8.00	3.69
1,1,1-trifluoropropan-2-ol	0	-4.16	-8.88	4.72	-0.0287	0.1095	3.50	-5.38	1.22
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-10.06	6.29	-0.0219	0.1219	3.99	-6.07	2.30
phenol	0	-6.62	-10.10	3.48	-0.0262	0.1151	3.72	-6.38	-0.24
p-bromophenol	0	-7.13	-11.01	3.88	-0.0240	0.1176	3.87	-7.14	0.01
o-cresol	0	-5.87	-9.55	3.68	-0.0264	0.1151	3.71	-5.84	-0.03
m-cresol	0	-5.49	-9.99	4.50	-0.0265	0.1161	3.70	-6.29	0.80
p-cresol	0	-6.14	-9.94	3.80	-0.0268	0.1158	3.68	-6.26	0.12

1,2-ethanediol	0	-9.30	-12.90	3.60	-0.0356	0.1104	2.59	-10.31	1.01
acetic acid	0	-6.70	-11.11	4.41	-0.0308	0.1239	3.32	-7.80	1.10
propanoic acid	0	-6.47	-10.81	4.34	-0.0299	0.1232	3.41	-7.40	0.93
butanoic acid	0	-6.36	-10.85	4.49	-0.0299	0.1234	3.41	-7.45	1.09
pentanoic acid	0	-6.16	-10.95	4.79	-0.0297	0.1238	3.43	-7.52	1.36
hexanoic acid	0	-6.21	-11.01	4.80	-0.0299	0.1227	3.40	-7.60	1.39
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-19.33	7.37	-0.0277	0.1266	3.63	-15.70	3.74
ammonia	0	-4.29	-7.88	3.59	-0.0421	0.0662	1.07	-6.81	2.52
methylamine	0	-4.56	-6.15	1.59	-0.0413	0.0636	1.30	-4.85	0.29
ethylamine	0	-4.50	-6.24	1.74	-0.0412	0.0625	1.32	-4.91	0.41
butylamine	0	-4.29	-6.36	2.07	-0.0410	0.0621	1.35	-5.01	0.72
propylamine	0	-4.39	-6.29	1.90	-0.0411	0.0625	1.34	-4.96	0.57
pentylamine	0	-4.10	-6.47	2.37	-0.0413	0.0621	1.29	-5.18	1.08
dimethylamine	0	-4.29	-4.53	0.24	-0.0393	0.0632	1.78	-2.75	-1.54
diethylamine	0	-4.07	-4.43	0.36	-0.0390	0.0607	1.86	-2.57	-1.50
dipropylamine	0	-3.66	-4.53	0.87	-0.0386	0.0605	1.93	-2.60	-1.06
trimethylamine	0	-3.23	-2.95	-0.28	-0.0369	0.0329	2.28	-0.68	-2.55
azetidine	0	-5.56	-4.91	-0.65	-0.0405	0.0623	1.49	-3.42	-2.14
pyrrolidine	0	-5.48	-5.26	-0.22	-0.0404	0.0614	1.51	-3.75	-1.73
piperidine	0	-5.11	-4.02	-1.09	-0.0384	0.0626	1.98	-2.03	-3.08
2-methoxyethanamine	0	-6.55	-9.57	3.02	-0.0398	0.0650	1.67	-7.89	1.34
1,2-ethanediamine	0	-9.72	-11.91	2.19	-0.0401	0.0647	1.60	-10.31	0.59
nitromethane	0	-3.95	-9.36	5.41	-0.0229	0.0587	3.86	-5.51	1.56
nitroethane	0	-3.71	-8.89	5.18	-0.0236	0.0544	3.82	-5.07	1.36
1-nitropropane	0	-3.34	-8.83	5.49	-0.0236	0.0538	3.82	-5.01	1.67
2-nitropropane	0	-3.14	-8.19	5.05	-0.0240	0.0511	3.80	-4.39	1.25
1-nitrobutane	0	-3.08	-8.91	5.83	-0.0236	0.0538	3.82	-5.09	2.01
nitrobenzene	0	-4.12	-8.53	4.41	-0.0235	0.0530	3.82	-4.71	0.59
2-methyl-1-nitrobenzene	0	-3.59	-8.20	4.61	-0.0248	0.0507	3.75	-4.45	0.86
pyridine	0	-4.70	-6.21	1.51	-0.0377	0.0477	2.13	-4.09	-0.61
2-methylpyridine	0	-4.63	-5.86	1.23	-0.0377	0.0459	2.12	-3.74	-0.89
3-methylpyridine	0	-4.77	-6.26	1.49	-0.0382	0.0454	2.01	-4.24	-0.53
4-methylpyridine	0	-4.94	-6.42	1.48	-0.0385	0.0442	1.95	-4.47	-0.47
4-ethylpyridine	0	-4.74	-6.44	1.70	-0.0385	0.0443	1.95	-4.49	-0.25
2,4-dimethylpyridine	0	-4.86	-6.06	1.20	-0.0385	0.0428	1.95	-4.11	-0.75

2,5-dimethylpyridine	0	-4.72	-5.89	1.17	-0.0381	0.0442	2.04	-3.84	-0.88
2,6-dimethylpyridine	0	-4.60	-5.56	0.96	-0.0377	0.0452	2.12	-3.44	-1.16
3,4-dimethylpyridine	0	-5.22	-6.59	1.37	-0.0390	0.0436	1.84	-4.75	-0.47
3,5-dimethylpyridine	0	-4.84	-6.30	1.46	-0.0388	0.0439	1.90	-4.40	-0.44
aniline	0	-5.49	-9.26	3.77	-0.0305	0.0791	3.27	-5.99	0.50
N-methylaniline	0	-4.68	-7.34	2.66	-0.0262	0.0783	3.66	-3.68	-1.00
2-methylaniline	0	-5.56	-8.67	3.11	-0.0310	0.0769	3.20	-5.47	-0.09
3-methylaniline	0	-5.67	-9.13	3.46	-0.0311	0.0783	3.20	-5.93	0.26
4-methylaniline	0	-5.55	-9.04	3.49	-0.0313	0.0767	3.17	-5.87	0.32
N-ethylaniline	0	-4.62	-7.20	2.58	-0.0232	0.0792	3.85	-3.35	-1.27
3-aminoaniline	0	-9.92	-14.81	4.89	-0.0312	0.0775	3.18	-11.63	1.71
N,N-dimethylaniline	0	-3.58	-5.47	1.89	-0.0207	0.0386	3.95	-1.52	-2.06
piperazine	0	-7.40	-7.50	0.10	-0.0381	0.0638	2.05	-5.45	-1.95
N-methylpiperazine	0	-7.77	-6.08	-1.69	-0.0377	0.0644	2.14	-3.94	-3.83
N,N'-dimethylpiperazine	0	-7.58	-4.63	-2.95	-0.0355	0.0328	2.54	-2.09	-5.49
1-methylthymine	0	-10.40	-17.60	7.20	-0.0354	0.1059	2.61	-15.00	4.60
9-methyladenine	0	-13.60	-16.32	2.72	-0.0403	0.0953	1.57	-14.75	1.15
acetamide	0	-9.71	-13.50	3.79	-0.0376	0.0935	2.17	-11.32	1.61
E-N-methylacetamide	0	-10.00	-11.89	1.89	-0.0391	0.0874	1.84	-10.05	0.05
Z-N-methylacetamide	0	-10.00	-11.36	1.36	-0.0394	0.0932	1.77	-9.58	-0.42
benzamide	0	-10.90	-13.94	3.04	-0.0370	0.0928	2.30	-11.64	0.74
2,6-dichlorothiobenzamide	0	-10.81	-16.04	5.23	-0.0241	0.1086	3.84	-12.19	1.38
urea	0	-13.80	-17.59	3.79	-0.0371	0.0910	2.28	-15.31	1.51
1,1-dimethyl-3-phenylurea	0	-9.63	-13.08	3.45	-0.0355	0.0876	2.56	-10.52	0.89
hydrazine	0	-6.26	-10.85	4.59	-0.0386	0.0668	1.93	-8.91	2.65
methylhydrazine	0	-5.31	-9.47	4.16	-0.0385	0.0674	1.96	-7.51	2.20
1,1-dimethylhydrazine	0	-4.48	-7.55	3.07	-0.0385	0.0682	1.96	-5.59	1.11
2-methylpyrazine	0	-5.57	-7.11	1.54	-0.0335	0.0471	2.87	-4.24	-1.33
2-ethylpyrazine	0	-5.51	-6.69	1.18	-0.0336	0.0470	2.85	-3.84	-1.67
morpholine	0	-7.17	-7.53	0.36	-0.0367	0.0666	2.34	-5.19	-1.98
N-methylmorpholine	0	-6.34	-5.97	-0.37	-0.0346	0.0365	2.70	-3.27	-3.07
acetonitrile	0	-3.89	-8.73	4.84	-0.0304	0.0555	3.27	-5.46	1.57
butanonitrile	0	-3.64	-8.10	4.46	-0.0304	0.0514	3.27	-4.83	1.19
propionitrile	0	-3.85	-8.31	4.46	-0.0305	0.0515	3.25	-5.06	1.21
benzonitrile	0	-4.10	-8.79	4.69	-0.0296	0.0516	3.34	-5.44	1.34

2,6-dichlorobenzonitrile	0	-5.22	-9.29	4.07	-0.0281	0.0556	3.50	-5.79	0.57
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-13.19	4.19	-0.0283	0.1054	3.52	-9.66	0.66
trimethylphosphate	0	-8.70	-12.62	3.92	-0.0344	0.0578	2.73	-9.90	1.20
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-12.23	5.62	-0.0305	0.0677	3.26	-8.97	2.36
phosphine	0	0.60	-1.47	2.07	-0.0121	0.0372	4.13	2.67	-2.07
hydrogen sulfide	0	-0.70	-4.44	3.74	-0.0142	0.0540	4.11	-0.33	-0.37
dimethyl sulfide	0	-1.54	-4.16	2.62	-0.0193	0.0422	4.00	-0.17	-1.37
diethyl sulfide	0	-1.43	-3.91	2.48	-0.0201	0.0359	3.97	0.06	-1.49
dipropyl sulfide	0	-1.27	-4.10	2.83	-0.0203	0.0355	3.97	-0.13	-1.14
bis(2-chloroethyl)sulfide	0	-3.92	-8.60	4.68	-0.0142	0.0490	4.11	-4.49	0.57
dimethyl disulfide	0	-1.83	-5.06	3.23	-0.0142	0.0455	4.11	-0.95	-0.88
diethyl disulfide	0	-1.63	-4.54	2.91	-0.0146	0.0422	4.10	-0.44	-1.19
methanethiol	0	-1.24	-4.27	3.03	-0.0173	0.0473	4.05	-0.21	-1.03
ethanethiol	0	-1.30	-4.16	2.86	-0.0174	0.0462	4.05	-0.10	-1.20
1-propanethiol	0	-1.05	-4.22	3.17	-0.0174	0.0461	4.05	-0.17	-0.88
thiophene	0	-1.42	-4.24	2.82	-0.0056	0.0524	4.16	-0.08	-1.34
thiophenol	0	-2.55	-6.08	3.53	-0.0114	0.0536	4.14	-1.94	-0.61
thioanisole	0	-2.73	-5.95	3.22	-0.0134	0.0461	4.12	-1.83	-0.90
tetramethylsilane	0	3.04	-1.73	4.77	0.0006	0.0320	4.16	2.43	0.61
acetylene	-1	-76.50	-70.41	-6.09	-0.0628	0.0348	-10.00	-80.41	3.91
acetonitrile	-1	-66.60	-63.30	-3.30	-0.0564	0.0169	-5.25	-68.55	1.95
cyanamide	-1	-72.20	-68.76	-3.44	-0.0566	0.0453	-5.38	-74.13	1.93
aniline	-1	-62.90	-58.66	-4.24	-0.0631	0.0231	-10.25	-68.91	6.01
diphenylamine	-1	-54.60	-50.62	-3.98	-0.0553	0.0271	-4.57	-55.19	0.59
hydrogen cyanide	-1	-70.20	-69.28	-0.92	-0.0553	-0.0323	-4.55	-73.82	3.62
formic acid	-1	-76.20	-68.81	-7.39	-0.0570	0.0091	-5.66	-74.47	-1.73
acetic acid	-1	-77.60	-68.53	-9.07	-0.0588	0.0222	-6.85	-75.38	-2.22
propanoic acid	-1	-76.20	-66.42	-9.78	-0.0588	0.0202	-6.83	-73.25	-2.95
hexanoic acid	-1	-74.60	-65.64	-8.96	-0.0588	0.0265	-6.86	-72.50	-2.10
acrylic acid	-1	-74.00	-67.01	-6.99	-0.0582	0.0325	-6.43	-73.44	-0.56
pyruvic acid	-1	-68.50	-66.50	-2.00	-0.0551	0.0363	-4.45	-70.96	2.46
benzoic acid	-1	-71.20	-64.23	-6.97	-0.0575	0.0352	-5.96	-70.19	-1.01
methanol	-1	-95.00	-72.02	-22.98	-0.0711	-0.0073	-18.45	-90.47	-4.53
ethanol	-1	-90.70	-68.39	-22.31	-0.0711	0.0145	-18.56	-86.96	-3.74
1-propanol	-1	-88.30	-67.83	-20.47	-0.0712	0.0208	-18.65	-86.48	-1.82

isopropanol	-1	-86.30	-65.58	-20.72	-0.0703	0.0146	-17.58	-83.16	-3.14
2-butanol	-1	-84.20	-62.39	-21.81	-0.0699	0.0144	-17.11	-79.49	-4.71
t-butanol	-1	-82.30	-63.48	-18.82	-0.0694	0.0145	-16.56	-80.04	-2.26
allyl alcohol	-1	-86.60	-67.42	-19.18	-0.0705	0.0245	-17.75	-85.17	-1.43
benzyl alcohol	-1	-85.10	-62.82	-22.28	-0.0693	0.0309	-16.40	-79.22	-5.88
2-methoxyethanol	-1	-89.40	-69.87	-19.53	-0.0708	0.0283	-18.19	-88.06	-1.34
phenol	-1	-71.90	-60.18	-11.72	-0.0619	0.0243	-9.19	-69.37	-2.53
2-methylphenol	-1	-70.20	-58.39	-11.81	-0.0622	0.0229	-9.45	-67.84	-2.36
3-methylphenol	-1	-71.10	-60.06	-11.04	-0.0622	0.0271	-9.52	-69.58	-1.52
4-methylphenol	-1	-72.00	-60.05	-11.95	-0.0626	0.0253	-9.83	-69.88	-2.12
1,2-ethanediol	-1	-85.30	-74.58	-10.72	-0.0710	0.0914	-18.35	-92.93	7.63
3-hydroxyphenol	-1	-73.80	-63.98	-9.82	-0.0612	0.1002	-8.63	-72.62	-1.18
4-hydroxyphenol	-1	-77.60	-65.83	-11.77	-0.0629	0.0986	-10.04	-75.86	-1.74
methyl hydroperoxide	-1	-93.20	-75.32	-17.88	-0.0707	0.0178	-18.07	-93.39	0.19
ethyl hydroperoxide	-1	-89.20	-74.72	-14.48	-0.0710	0.0261	-18.35	-93.07	3.87
acetaldehyde	-1	-76.50	-65.35	-11.15	-0.0632	0.0134	-10.30	-75.65	-0.85
acetone	-1	-76.20	-64.11	-12.09	-0.0636	0.0192	-10.72	-74.83	-1.37
3-pentanone	-1	-73.70	-58.90	-14.80	-0.0623	0.0188	-9.54	-68.43	-5.27
water	-1	-104.70	-85.30	-19.40	-0.0765	0.0244	-25.77	-111.07	6.37
hydrogen peroxide	-1	-97.30	-82.64	-14.66	-0.0712	0.0724	-18.64	-101.27	3.97
hydroperoxyl radical	-1	-83.30	-75.93	-7.37	-0.0611	-0.0400	-8.57	-84.50	1.20
2-nitrophenol	-1	-60.10	-58.21	-1.89	-0.0545	0.0353	-4.10	-62.31	2.21
3-nitrophenol	-1	-61.90	-54.88	-7.02	-0.0580	0.0385	-6.26	-61.15	-0.75
4-nitrophenol	-1	-57.80	-53.11	-4.69	-0.0523	0.0379	-2.90	-56.01	-1.79
nitromethane	-1	-76.50	-66.51	-9.99	-0.0558	0.0285	-4.86	-71.38	-5.12
4-nitroaniline	-1	-57.40	-53.62	-3.78	-0.0528	0.0400	-3.15	-56.77	-0.63
acetamide	-1	-80.20	-66.53	-13.67	-0.0604	0.0240	-8.01	-74.54	-5.66
methanethiol	-1	-73.80	-66.07	-7.73	-0.0492	0.0160	-1.46	-67.52	-6.28
ethanethiol	-1	-71.80	-63.67	-8.13	-0.0487	0.0216	-1.24	-64.91	-6.89
1-propanethiol	-1	-70.50	-63.56	-6.94	-0.0488	0.0244	-1.25	-64.81	-5.69
thiophenol	-1	-63.40	-57.71	-5.69	-0.0437	0.0308	0.59	-57.12	-6.28
hydrogen sulfide	-1	-72.10	-67.15	-4.95	-0.0480	0.0079	-0.93	-68.08	-4.02
dimethyl sulfoxide	-1	-67.70	-62.59	-5.11	-0.0607	0.0294	-8.27	-70.87	3.17
hydrofluoric acid	-1	-104.40	-89.91	-14.49	-0.0778	-0.0778	-27.72	-117.63	13.23
hydrochloric acid	-1	-74.50	-70.97	-3.53	-0.0453	-0.0453	0.07	-70.90	-3.60

hydrobromic acid	-1	-68.30	-66.13	-2.17	-0.0381	-0.0381	2.04	-64.09	-4.21
chloroform	-1	-54.10	-51.60	-2.50	-0.0444	0.0093	0.36	-51.23	-2.87
trifluoroacetic acid	-1	-59.30	-60.49	1.19	-0.0513	0.0495	-2.40	-62.90	3.60
chloroacetic acid	-1	-69.70	-63.37	-6.33	-0.0540	0.0355	-3.83	-67.19	-2.51
dichloroacetic acid	-1	-62.30	-59.32	-2.98	-0.0510	0.0449	-2.27	-61.59	-0.71
2,2,2-trifluoroethanol	-1	-77.50	-63.78	-13.72	-0.0667	0.0289	-13.60	-77.38	-0.12
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-58.38	-7.12	-0.0618	0.0373	-9.16	-67.54	2.04
2-chlorophenol	-1	-66.10	-57.46	-8.64	-0.0595	0.0315	-7.37	-64.83	-1.27
4-chlorophenol	-1	-66.00	-55.93	-10.07	-0.0600	0.0313	-7.71	-63.64	-2.36
methylamine	1	-76.40	-83.18	6.78	0.0319	0.1359	4.29	-78.89	2.49
n-propylamine	1	-71.50	-78.20	6.70	0.0070	0.1351	4.29	-73.91	2.41
isopropylamine	1	-69.60	-76.48	6.88	0.0078	0.1329	4.28	-72.20	2.60
tert-butylamine	1	-67.30	-73.84	6.54	0.0085	0.1318	4.28	-69.57	2.27
cyclohexanamine	1	-68.70	-73.33	4.63	0.0066	0.1324	4.28	-69.05	0.35
allylamine	1	-72.00	-78.88	6.88	-0.0124	0.1370	4.27	-74.61	2.61
dimethylamine	1	-68.60	-74.83	6.23	0.0301	0.1312	4.28	-70.56	1.96
diethylamine	1	-63.40	-68.64	5.24	0.0076	0.1253	4.26	-64.39	0.99
di-n-propylamine	1	-60.50	-66.48	5.98	0.0125	0.1254	4.26	-62.22	1.72
diallylamine	1	-61.60	-68.03	6.43	-0.0107	0.1281	4.25	-63.78	2.18
trimethylamine	1	-61.10	-67.46	6.36	0.0293	0.1279	4.27	-63.20	2.10
triethylamine	1	-54.60	-59.52	4.92	0.0094	0.1148	4.23	-55.29	0.69
aniline	1	-72.40	-78.84	6.44	0.0072	0.1412	4.31	-74.52	2.12
2-methylaniline	1	-70.30	-76.59	6.29	0.0047	0.1392	4.31	-72.29	1.99
3-methylaniline	1	-69.60	-76.97	7.37	0.0054	0.1414	4.32	-72.66	3.06
4-methylaniline	1	-69.80	-76.93	7.13	0.0066	0.1409	4.31	-72.61	2.81
3-aminoaniline	1	-65.80	-80.62	14.82	-0.0179	0.1399	4.19	-76.43	10.63
N-methylaniline	1	-62.60	-70.37	7.77	0.0070	0.1346	4.29	-66.08	3.48
N-ethylaniline	1	-62.20	-67.41	5.21	0.0068	0.1308	4.27	-63.14	0.94
N,N-dimethylaniline	1	-57.20	-62.92	5.72	0.0071	0.1269	4.26	-58.66	1.46
4-methyl-N,N-dimethylaniline	1	-55.90	-61.26	5.36	0.0066	0.1251	4.26	-57.00	1.10
N,N-diethylaniline	1	-54.00	-58.32	4.32	0.0067	0.1193	4.24	-54.08	0.08
1-aminonaphthalene	1	-67.40	-75.64	8.24	0.0037	0.1426	4.32	-71.32	3.92
aziridine	1	-70.90	-76.84	5.94	0.0297	0.1389	4.31	-72.53	1.63
azetidine	1	-67.70	-72.49	4.79	0.0204	0.1304	4.27	-68.21	0.51
pyrrolidine	1	-66.00	-70.19	4.19	0.0133	0.1294	4.27	-65.92	-0.08

piperidine	1	-64.20	-68.42	4.22	0.0093	0.1307	4.27	-64.14	-0.06
azacycloheptane	1	-63.30	-66.84	3.54	0.0011	0.1304	4.27	-62.57	-0.73
pyrrole	1	-61.40	-68.19	6.79	0.0175	0.1377	4.30	-63.89	2.49
pyridine	1	-61.10	-66.61	5.51	0.0232	0.1405	4.31	-62.30	1.20
quinoline	1	-56.00	-60.73	4.73	0.0100	0.1332	4.28	-56.44	0.44
piperazine	1	-66.00	-71.91	5.91	-0.0273	0.1315	3.68	-68.23	2.23
acetonitrile	1	-75.30	-77.50	2.20	0.0393	0.1847	4.59	-72.91	-2.39
ammonia	1	-85.20	-93.46	8.26	0.0669	0.1427	4.32	-89.14	3.94
hydrazine	1	-84.60	-93.61	9.01	-0.0145	0.1421	4.26	-89.35	4.75
methanol	1	-93.00	-91.99	-1.01	0.0142	0.1948	4.69	-87.30	-5.70
ethanol	1	-88.40	-86.16	-2.24	-0.0027	0.1925	4.67	-81.49	-6.91
dimethyl ether	1	-79.70	-77.34	-2.36	0.0110	0.1872	4.62	-72.72	-6.98
diethyl ether	1	-71.50	-68.84	-2.66	0.0065	0.1733	4.50	-64.34	-7.16
acetone	1	-77.10	-74.85	-2.25	0.0062	0.1729	4.50	-70.36	-6.74
acetophenone	1	-64.50	-62.89	-1.61	0.0020	0.1484	4.35	-58.54	-5.96
water	1	-110.30	-111.14	0.84	0.0190	0.2079	4.84	-106.30	-4.00
4-methoxyaniline	1	-71.20	-78.17	6.97	-0.0210	0.1390	4.09	-74.08	2.88
4-nitroaniline	1	-75.90	-92.54	16.64	-0.0175	0.1450	4.22	-88.32	12.42
morpholine	1	-69.60	-76.28	6.68	-0.0207	0.1348	4.08	-72.20	2.60
acetamide	1	-73.90	-81.73	7.83	-0.0005	0.1646	4.44	-77.29	3.39
benzamide	1	-67.20	-73.66	6.46	-0.0023	0.1611	4.42	-69.24	2.04
dimethyl sulfide	1	-64.50	-69.87	5.37	0.0251	0.0958	4.19	-65.68	1.18
dimethyl sulfoxide	1	-67.70	-73.14	5.44	-0.0058	0.1585	4.40	-68.74	1.04
3-chloroaniline	1	-74.70	-82.04	7.34	-0.0017	0.1432	4.32	-77.71	3.01
4-chloroaniline	1	-74.10	-82.38	8.28	0.0001	0.1435	4.32	-78.06	3.96
PEARSON			0.99					1.00	

Table S 5-1

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/G3large method for the cavity surface with constant density = 0.0005 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.04	2.04	-0.0016	0.0119	1.14	1.11	0.89
ethane	0	1.83	0.17	1.66	-0.0020	0.0102	1.15	1.32	0.51
n-propane	0	1.96	0.28	1.68	-0.0022	0.0100	1.15	1.43	0.53
n-butane	0	2.08	0.40	1.68	-0.0023	0.0101	1.15	1.55	0.53
n-pentane	0	2.33	0.52	1.81	-0.0024	0.0100	1.15	1.67	0.66
n-hexane	0	2.49	0.65	1.84	-0.0025	0.0100	1.15	1.80	0.69
n-heptane	0	2.62	-0.36	2.98	-0.0025	0.0097	1.15	0.79	1.83
n-octane	0	2.89	-0.39	3.28	-0.0026	0.0097	1.15	0.76	2.13
2-methylpropane	0	2.32	0.33	1.99	-0.0023	0.0100	1.15	1.48	0.84
2,2-dimethylpropane	0	2.50	0.37	2.13	-0.0022	0.0101	1.15	1.52	0.98
2-methylpentane	0	2.52	-0.34	2.86	-0.0026	0.0102	1.15	0.81	1.71
2,4-dimethylpentane	0	2.88	-0.42	3.30	-0.0026	0.0105	1.15	0.73	2.15
2,2,4-trimethylpentane	0	2.85	-0.50	3.35	-0.0026	0.0116	1.14	0.65	2.20
cyclopropane	0	0.75	-0.25	1.00	-0.0086	0.0134	1.07	0.83	-0.08
cyclopentane	0	1.20	0.57	0.63	-0.0028	0.0096	1.15	1.72	-0.52
cyclohexane	0	1.23	-0.22	1.45	-0.0026	0.0089	1.15	0.93	0.30
methylcyclohexane	0	1.71	-0.29	2.00	-0.0026	0.0097	1.15	0.86	0.85
cis-1,2-dimethylcyclohexane	0	1.58	-0.34	1.92	-0.0026	0.0106	1.15	0.81	0.77
ethene	0	1.27	-0.70	1.97	-0.0110	0.0170	0.98	0.28	0.99
propene	0	1.27	-0.51	1.78	-0.0117	0.0156	0.96	0.45	0.82
1-butene	0	1.38	-0.30	1.68	-0.0119	0.0150	0.95	0.65	0.73
1-pentene	0	1.66	-0.20	1.86	-0.0120	0.0148	0.95	0.75	0.91
E-2-pentene	0	1.34	-0.08	1.42	-0.0117	0.0137	0.96	0.89	0.45
1-hexene	0	1.68	-0.13	1.81	-0.0119	0.0151	0.95	0.82	0.86
2-methylpropene	0	1.16	-0.38	1.54	-0.0122	0.0136	0.94	0.57	0.59
s-trans-1,3-butadiene	0	0.61	-1.13	1.74	-0.0098	0.0174	1.02	-0.11	0.72
cyclopentene	0	0.56	0.03	0.53	-0.0120	0.0159	0.94	0.97	-0.41
ethyne	0	-0.01	-2.84	2.83	-0.0115	0.0397	0.45	-2.39	2.38
propyne	0	-0.31	-2.14	1.83	-0.0134	0.0354	0.52	-1.62	1.31
1-butyne	0	-0.16	-1.87	1.71	-0.0136	0.0353	0.51	-1.36	1.20
1-pentyne	0	0.01	-1.61	1.62	-0.0137	0.0349	0.51	-1.10	1.11
1-hexyne	0	0.29	-1.64	1.93	-0.0137	0.0345	0.52	-1.11	1.40

butenyne	0	0.04	-2.34	2.38	-0.0128	0.0372	0.49	-1.86	1.90
benzene	0	-0.87	-1.33	0.46	-0.0073	0.0181	1.07	-0.26	-0.61
ethylbenzene	0	-0.80	-2.18	1.38	-0.0083	0.0174	1.06	-1.12	0.32
naphthalene	0	-2.39	-3.24	0.85	-0.0074	0.0185	1.06	-2.17	-0.22
anthracene	0	-4.23	-4.19	-0.04	-0.0074	0.0187	1.06	-3.12	-1.11
toluene	0	-0.89	-2.16	1.27	-0.0083	0.0175	1.06	-1.11	0.22
p-xylene	0	-0.81	-2.04	1.23	-0.0089	0.0161	1.05	-0.99	0.18
m-xylene	0	-0.84	-2.07	1.23	-0.0091	0.0170	1.04	-1.03	0.19
o-xylene	0	-0.90	-2.16	1.26	-0.0091	0.0166	1.04	-1.12	0.22
fluoromethane	0	-0.22	-1.60	1.38	-0.0193	0.0198	0.28	-1.32	1.10
chloromethane	0	-0.56	-0.63	0.07	-0.0104	0.0222	0.95	0.32	-0.88
bromomethane	0	-0.82	-0.72	-0.10	-0.0089	0.0231	0.98	0.26	-1.08
chlorofluoromethane	0	-0.77	-0.85	0.08	-0.0126	0.0298	0.72	-0.14	-0.63
dichloromethane	0	-1.36	0.23	-1.59	-0.0064	0.0307	0.89	1.12	-2.48
dibromomethane	0	-2.11	0.08	-2.19	-0.0052	0.0313	0.88	0.96	-3.07
chlorodifluoromethane	0	-0.50	0.46	-0.96	-0.0078	0.0385	0.62	1.08	-1.58
chloroform	0	-1.07	2.27	-3.34	-0.0035	0.0372	0.71	2.98	-4.05
chloroethane	0	-0.63	-0.44	-0.19	-0.0112	0.0207	0.94	0.49	-1.12
bromoethane	0	-0.70	-0.57	-0.13	-0.0096	0.0216	0.98	0.41	-1.11
bromoform	0	-1.98	-2.49	0.51	-0.0029	0.0369	0.72	-1.76	-0.22
tetrafluoromethane	0	3.16	2.95	0.21	-0.0026	0.0381	0.68	3.63	-0.47
difluorodichloromethane	0	1.69	4.09	-2.40	-0.0039	0.0246	1.03	5.12	-3.43
fluorotrichloromethane	0	0.82	4.56	-3.74	-0.0046	0.0250	1.02	5.58	-4.76
bromotrifluoromethane	0	1.79	3.32	-1.53	-0.0034	0.0370	0.72	4.04	-2.25
bromotrichloromethane	0	-0.93	-1.16	0.23	-0.0015	0.0273	0.99	-0.18	-0.75
hexafluoroethane	0	3.94	-0.89	4.83	-0.0027	0.0383	0.67	-0.22	4.16
hexachloroethane	0	-1.40	-1.45	0.05	-0.0032	0.0234	1.05	-0.40	-1.00
chloropentafluoroethane	0	2.86	-0.91	3.77	-0.0035	0.0365	0.74	-0.17	3.03
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.16	2.93	-0.0054	0.0254	1.01	-0.16	1.93
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-3.20	3.72	-0.0082	0.0396	0.56	-2.64	3.16
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-2.86	2.73	-0.0058	0.0387	0.64	-2.22	2.09
1-chloro-2,2,2-trifluoroethane	0	0.06	0.89	-0.83	-0.0074	0.0319	0.84	1.73	-1.67
1,1,1,2-tetrachloroethane	0	-1.15	-2.74	1.59	-0.0064	0.0302	0.90	-1.84	0.69
1,1,1-trichloroethane	0	-0.25	-1.93	1.68	-0.0047	0.0221	1.06	-0.88	0.63
1,1,2-trichloroethane	0	-1.95	-3.41	1.46	-0.0070	0.0324	0.84	-2.57	0.62

1,1-difluoroethane	0	-0.11	-1.41	1.30	-0.0150	0.0260	0.64	-0.77	0.66
1-bromo-2-chloroethane	0	-1.95	0.22	-2.17	-0.0082	0.0254	0.97	1.18	-3.13
octafluoropropane	0	4.28	-1.04	5.32	-0.0026	0.0383	0.67	-0.37	4.65
2-chloropropane	0	-0.25	-0.30	0.05	-0.0118	0.0197	0.92	0.62	-0.87
1-chloropropane	0	-0.27	-0.26	-0.01	-0.0113	0.0201	0.94	0.68	-0.95
1-bromopropane	0	-0.56	-2.28	1.72	-0.0097	0.0211	0.98	-1.29	0.73
2-bromopropane	0	-0.48	-2.27	1.79	-0.0102	0.0208	0.97	-1.30	0.82
2-chlorobutane	0	0.07	-2.11	2.18	-0.0119	0.0191	0.92	-1.19	1.26
1-bromobutane	0	-0.41	-0.29	-0.12	-0.0098	0.0210	0.98	0.69	-1.10
1-chloropentane	0	0.07	-2.35	2.42	-0.0114	0.0199	0.93	-1.42	1.49
2-chloropentane	0	0.07	-2.12	2.19	-0.0119	0.0190	0.92	-1.20	1.27
1-bromopentane	0	-0.08	-2.36	2.28	-0.0099	0.0210	0.98	-1.38	1.30
1-bromo-isobutane	0	-0.03	-2.15	2.12	-0.0098	0.0210	0.98	-1.17	1.14
tetrachloroethene	0	0.05	5.15	-5.10	-0.0036	0.0226	1.06	6.20	-6.15
trichloroethene	0	-0.39	2.99	-3.38	-0.0052	0.0333	0.83	3.82	-4.21
chloroethene	0	-0.59	-0.13	-0.46	-0.0084	0.0263	0.94	0.82	-1.41
E-1,2-dichloroethene	0	-0.76	1.28	-2.04	-0.0057	0.0302	0.91	2.19	-2.95
Z-1,2-dichloroethene	0	-1.17	0.56	-1.73	-0.0071	0.0308	0.88	1.43	-2.60
3-chloropropene	0	-0.57	-0.64	0.07	-0.0101	0.0224	0.96	0.31	-0.88
3-bromopropene	0	-0.86	-1.07	0.21	-0.0094	0.0237	0.96	-0.11	-0.75
fluorobenzene	0	-0.78	-2.73	1.95	-0.0148	0.0218	0.72	-2.02	1.24
chlorobenzene	0	-1.12	-0.13	-0.99	-0.0080	0.0217	1.02	0.89	-2.01
bromobenzene	0	-1.46	-2.55	1.09	-0.0069	0.0220	1.04	-1.51	0.05
1,4-dichlorobenzene	0	-1.01	-2.50	1.49	-0.0065	0.0246	1.01	-1.49	0.48
1,2-dichlorobenzene	0	-1.36	1.08	-2.44	-0.0082	0.0242	0.98	2.07	-3.43
p-dibromobenzene	0	-2.30	-2.59	0.29	-0.0057	0.0246	1.02	-1.58	-0.72
chlorotoluene	0	-1.92	-4.07	2.15	-0.0112	0.0227	0.91	-3.16	1.24
o-chlorotoluene	0	-1.15	-2.28	1.13	-0.0084	0.0213	1.02	-1.26	0.11
bromotoluene	0	-2.37	-4.07	1.70	-0.0097	0.0238	0.95	-3.12	0.75
p-bromotoluene	0	-1.39	-2.54	1.15	-0.0074	0.0216	1.04	-1.51	0.12
2,3-dichlorobiphenyl	0	-2.45	-3.91	1.46	-0.0086	0.0236	0.98	-2.93	0.48
2,2'-dichlorobiphenyl	0	-2.73	-4.24	1.51	-0.0086	0.0217	1.01	-3.23	0.50
2,2',3'-trichlorobiphenyl	0	-1.99	-4.10	2.11	-0.0083	0.0240	0.98	-3.12	1.13
1,2-dimethoxyethane	0	-4.84	-1.93	-2.91	-0.0248	0.0142	-0.64	-2.57	-2.27
anisole	0	-2.45	-3.49	1.04	-0.0220	0.0195	-0.13	-3.62	1.17

dimethyl ether	0	-1.92	-1.61	-0.31	-0.0261	0.0142	-0.95	-2.56	0.64
diethyl ether	0	-1.76	-1.34	-0.42	-0.0270	0.0134	-1.17	-2.51	0.75
isopropyl ether	0	-0.53	-2.15	1.62	-0.0271	0.0139	-1.20	-3.35	2.82
methyl propyl ether	0	-1.66	-1.15	-0.51	-0.0260	0.0135	-0.90	-2.05	0.39
methyl isopropyl ether	0	-2.01	-2.14	0.13	-0.0262	0.0134	-0.96	-3.10	1.09
t-butyl methyl ether	0	-2.21	-2.10	-0.11	-0.0263	0.0132	-0.99	-3.09	0.88
ethyl phenyl ether	0	-2.22	-3.35	1.13	-0.0219	0.0193	-0.11	-3.45	1.23
tetrahydrofuran	0	-3.47	-1.57	-1.90	-0.0276	0.0137	-1.33	-2.90	-0.57
tetrahydropyran	0	-3.12	-2.38	-0.74	-0.0272	0.0124	-1.21	-3.59	0.47
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-4.06	3.94	-0.0161	0.0283	0.50	-3.55	3.43
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-4.83	4.94	-0.0103	0.0390	0.53	-4.31	4.42
acetaldehyde	0	-3.50	-4.45	0.95	-0.0267	0.0241	-1.19	-5.64	2.14
propanal	0	-3.44	-3.91	0.47	-0.0271	0.0233	-1.26	-5.18	1.74
butanal	0	-3.18	-3.95	0.77	-0.0269	0.0227	-1.22	-5.17	1.99
pentanal	0	-3.03	-4.82	1.79	-0.0271	0.0227	-1.26	-6.08	3.05
octanal	0	-2.29	-4.92	2.63	-0.0272	0.0220	-1.29	-6.20	3.91
benzaldehyde	0	-4.02	-5.76	1.74	-0.0275	0.0238	-1.39	-7.14	3.12
p-hydroxybenzaldehyde	0	-10.48	-9.48	-1.00	-0.0284	0.0651	-4.04	-13.52	3.04
m-hydroxybenzaldehyde	0	-9.51	-9.00	-0.51	-0.0272	0.0648	-3.66	-12.66	3.15
acetone	0	-3.85	-4.41	0.56	-0.0280	0.0208	-1.51	-5.92	2.07
2-butanone	0	-3.64	-3.86	0.22	-0.0283	0.0201	-1.56	-5.43	1.79
2-pentanone	0	-3.53	-4.86	1.33	-0.0284	0.0203	-1.60	-6.46	2.93
3-pentanone	0	-3.41	-4.44	1.03	-0.0278	0.0198	-1.43	-5.87	2.46
2-hexanone	0	-3.29	-4.90	1.61	-0.0284	0.0201	-1.61	-6.51	3.22
2-heptanone	0	-3.04	-4.94	1.90	-0.0284	0.0197	-1.61	-6.55	3.51
4-heptanone	0	-2.93	-4.47	1.54	-0.0280	0.0195	-1.48	-5.95	3.02
2-octanone	0	-2.88	-4.97	2.09	-0.0285	0.0197	-1.62	-6.59	3.71
5-nonanone	0	-2.67	-4.55	1.88	-0.0280	0.0193	-1.49	-6.04	3.37
3,3-dimethylbutanone	0	-2.89	-4.60	1.71	-0.0284	0.0189	-1.58	-6.17	3.28
cyclopentanone	0	-4.68	-5.35	0.67	-0.0283	0.0208	-1.58	-6.93	2.25
acetophenone	0	-4.58	-5.69	1.11	-0.0284	0.0222	-1.62	-7.31	2.73
methyl formate	0	-2.78	-3.69	0.91	-0.0253	0.0297	-0.95	-4.64	1.86
ethyl formate	0	-2.65	-3.49	0.84	-0.0256	0.0293	-1.01	-4.50	1.85
methyl acetate	0	-3.32	-3.35	0.03	-0.0268	0.0232	-1.21	-4.55	1.23
ethyl acetate	0	-3.10	-4.49	1.39	-0.0271	0.0227	-1.28	-5.77	2.67

propyl acetate	0	-2.86	-4.50	1.64	-0.0271	0.0221	-1.26	-5.76	2.90
butyl acetate	0	-2.55	-4.55	2.00	-0.0272	0.0225	-1.29	-5.84	3.29
methyl propanoate	0	-2.93	-2.89	-0.04	-0.0265	0.0226	-1.12	-4.01	1.08
methyl butanoate	0	-2.83	-4.26	1.43	-0.0266	0.0227	-1.15	-5.40	2.57
methyl pentanoate	0	-2.57	-4.30	1.73	-0.0266	0.0222	-1.14	-5.44	2.87
methyl hexanoate	0	-2.49	-4.33	1.84	-0.0267	0.0222	-1.16	-5.49	3.00
methyl benzoate	0	-3.91	-4.80	0.89	-0.0266	0.0217	-1.13	-5.93	2.02
hydrogen	0	2.33	-0.16	2.49	-0.0021	0.0139	1.14	0.98	1.35
water	0	-6.31	-5.57	-0.74	-0.0258	0.0566	-2.47	-8.04	1.73
water dimer	0	-11.27	-8.85	-2.42	-0.0294	0.0631	-4.13	-12.98	1.71
hydrogen peroxide	0	-8.58	-5.99	-2.59	-0.0214	0.0649	-2.45	-8.44	-0.14
methyl peroxide	0	-5.28	-4.20	-1.08	-0.0223	0.0633	-2.41	-6.60	1.32
ethyl peroxide	0	-5.32	-4.02	-1.30	-0.0227	0.0623	-2.38	-6.39	1.07
1,4-dioxane	0	-5.05	-2.56	-2.49	-0.0254	0.0164	-0.79	-3.34	-1.71
methanol	0	-5.11	-3.67	-1.44	-0.0263	0.0534	-2.31	-5.98	0.87
ethanol	0	-5.01	-3.25	-1.76	-0.0262	0.0523	-2.20	-5.45	0.44
1-propanol	0	-4.83	-3.10	-1.73	-0.0262	0.0512	-2.14	-5.24	0.41
isopropanol	0	-4.76	-3.05	-1.71	-0.0269	0.0486	-2.14	-5.19	0.43
1-butanol	0	-4.72	-2.98	-1.74	-0.0263	0.0509	-2.14	-5.12	0.40
t-butanol	0	-4.51	-2.74	-1.77	-0.0267	0.0478	-2.03	-4.77	0.26
1-pentanol	0	-4.47	-4.19	-0.28	-0.0268	0.0501	-2.22	-6.41	1.94
1-hexanol	0	-4.36	-4.22	-0.14	-0.0269	0.0494	-2.19	-6.41	2.05
1-heptanol	0	-4.24	-4.21	-0.03	-0.0269	0.0491	-2.18	-6.39	2.15
1-octanol	0	-4.09	-4.31	0.22	-0.0268	0.0494	-2.15	-6.46	2.37
allyl alcohol	0	-5.08	-3.27	-1.81	-0.0261	0.0518	-2.14	-5.42	0.34
cyclopentanol	0	-5.49	-3.70	-1.79	-0.0270	0.0464	-2.02	-5.72	0.23
2-methoxyethanol	0	-6.77	-4.37	-2.40	-0.0257	0.0535	-2.19	-6.56	-0.21
2,2,2-trifluoroethanol	0	-4.31	-7.07	2.76	-0.0201	0.0635	-2.08	-9.14	4.83
1,1,1-trifluoropropan-2-ol	0	-4.16	-4.68	0.52	-0.0223	0.0581	-1.88	-6.56	2.40
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-5.26	1.49	-0.0172	0.0677	-2.25	-7.50	3.73
phenol	0	-6.62	-4.27	-2.35	-0.0214	0.0606	-1.97	-6.24	-0.38
p-bromophenol	0	-7.13	-5.99	-1.14	-0.0198	0.0621	-1.89	-7.88	0.75
o-cresol	0	-5.87	-5.07	-0.80	-0.0209	0.0597	-1.80	-6.87	1.00
m-cresol	0	-5.49	-5.45	-0.04	-0.0218	0.0603	-2.00	-7.45	1.96
p-cresol	0	-6.14	-5.40	-0.74	-0.0220	0.0597	-1.99	-7.39	1.25

1,2-ethanediol	0	-9.30	-5.78	-3.52	-0.0277	0.0577	-3.06	-8.83	-0.47
acetic acid	0	-6.70	-5.25	-1.45	-0.0260	0.0668	-3.60	-8.85	2.15
propanoic acid	0	-6.47	-4.78	-1.69	-0.0257	0.0666	-3.50	-8.29	1.82
butanoic acid	0	-6.36	-4.62	-1.74	-0.0258	0.0661	-3.46	-8.09	1.73
pentanoic acid	0	-6.16	-6.07	-0.09	-0.0258	0.0660	-3.47	-9.54	3.38
hexanoic acid	0	-6.21	-6.10	-0.11	-0.0259	0.0663	-3.51	-9.62	3.41
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-9.95	-2.01	-0.0228	0.0689	-3.19	-13.14	1.18
ammonia	0	-4.29	-3.29	-1.00	-0.0276	0.0309	-1.56	-4.85	0.56
methylamine	0	-4.56	-2.42	-2.14	-0.0273	0.0290	-1.43	-3.85	-0.71
ethylamine	0	-4.50	-2.31	-2.19	-0.0275	0.0281	-1.47	-3.79	-0.71
butylamine	0	-4.29	-3.02	-1.27	-0.0277	0.0279	-1.51	-4.52	0.23
propylamine	0	-4.39	-2.20	-2.19	-0.0276	0.0281	-1.50	-3.70	-0.69
pentylamine	0	-4.10	-3.05	-1.05	-0.0278	0.0273	-1.53	-4.58	0.48
dimethylamine	0	-4.29	-1.52	-2.77	-0.0262	0.0286	-1.15	-2.67	-1.62
diethylamine	0	-4.07	-1.18	-2.89	-0.0261	0.0267	-1.08	-2.26	-1.81
dipropylamine	0	-3.66	-2.11	-1.55	-0.0260	0.0266	-1.04	-3.15	-0.51
trimethylamine	0	-3.23	-0.62	-2.61	-0.0250	0.0120	-0.66	-1.29	-1.94
azetidine	0	-5.56	-1.60	-3.96	-0.0274	0.0274	-1.44	-3.03	-2.53
pyrrolidine	0	-5.48	-2.56	-2.92	-0.0275	0.0272	-1.45	-4.01	-1.47
piperidine	0	-5.11	-1.79	-3.32	-0.0258	0.0277	-1.01	-2.81	-2.30
2-methoxyethanamine	0	-6.55	-3.70	-2.85	-0.0267	0.0300	-1.30	-5.00	-1.55
1,2-ethanediamine	0	-9.72	-4.74	-4.98	-0.0268	0.0296	-1.30	-6.04	-3.68
nitromethane	0	-3.95	-5.71	1.76	-0.0210	0.0308	-0.14	-5.86	1.91
nitroethane	0	-3.71	-5.12	1.41	-0.0217	0.0282	-0.20	-5.32	1.61
1-nitropropane	0	-3.34	-4.84	1.50	-0.0217	0.0277	-0.19	-5.04	1.70
2-nitropropane	0	-3.14	-4.38	1.24	-0.0221	0.0268	-0.24	-4.62	1.48
1-nitrobutane	0	-3.08	-6.31	3.23	-0.0218	0.0276	-0.20	-6.51	3.43
nitrobenzene	0	-4.12	-5.67	1.55	-0.0211	0.0266	-0.07	-5.74	1.62
2-methyl-1-nitrobenzene	0	-3.59	-5.33	1.74	-0.0221	0.0248	-0.20	-5.53	1.94
pyridine	0	-4.70	-3.78	-0.92	-0.0271	0.0236	-1.28	-5.06	0.36
2-methylpyridine	0	-4.63	-3.42	-1.21	-0.0272	0.0225	-1.29	-4.71	0.08
3-methylpyridine	0	-4.77	-3.78	-0.99	-0.0275	0.0221	-1.38	-5.16	0.39
4-methylpyridine	0	-4.94	-2.79	-2.15	-0.0279	0.0199	-1.45	-4.24	-0.70
4-ethylpyridine	0	-4.74	-3.88	-0.86	-0.0279	0.0200	-1.47	-5.35	0.61
2,4-dimethylpyridine	0	-4.86	-3.52	-1.34	-0.0279	0.0188	-1.46	-4.98	0.12

2,5-dimethylpyridine	0	-4.72	-3.40	-1.32	-0.0275	0.0213	-1.37	-4.76	0.04
2,6-dimethylpyridine	0	-4.60	-3.07	-1.53	-0.0272	0.0220	-1.28	-4.35	-0.25
3,4-dimethylpyridine	0	-5.22	-3.98	-1.24	-0.0282	0.0196	-1.55	-5.53	0.31
3,5-dimethylpyridine	0	-4.84	-3.78	-1.06	-0.0279	0.0211	-1.48	-5.26	0.42
aniline	0	-5.49	-5.01	-0.48	-0.0211	0.0384	-0.41	-5.42	-0.07
N-methylaniline	0	-4.68	-4.05	-0.63	-0.0187	0.0377	-0.04	-4.09	-0.59
2-methylaniline	0	-5.56	-4.56	-1.00	-0.0214	0.0369	-0.40	-4.96	-0.60
3-methylaniline	0	-5.67	-4.88	-0.79	-0.0213	0.0375	-0.41	-5.29	-0.38
4-methylaniline	0	-5.55	-4.82	-0.73	-0.0218	0.0370	-0.46	-5.28	-0.27
N-ethylaniline	0	-4.62	-3.93	-0.69	-0.0167	0.0380	0.16	-3.77	-0.85
3-aminoaniline	0	-9.92	-7.76	-2.16	-0.0213	0.0380	-0.41	-8.17	-1.75
N,N-dimethylaniline	0	-3.58	-3.16	-0.42	-0.0156	0.0166	0.70	-2.45	-1.13
piperazine	0	-7.40	-3.28	-4.12	-0.0255	0.0283	-0.97	-4.25	-3.15
N-methylpiperazine	0	-7.77	-2.65	-5.12	-0.0255	0.0286	-0.96	-3.61	-4.16
N,N'-dimethylpiperazine	0	-7.58	-1.99	-5.59	-0.0240	0.0121	-0.46	-2.45	-5.13
1-methylthymine	0	-10.40	-10.91	0.51	-0.0287	0.0548	-3.09	-14.01	3.61
9-methyladenine	0	-13.60	-8.64	-4.96	-0.0267	0.0471	-2.00	-10.64	-2.96
acetamide	0	-9.71	-7.50	-2.21	-0.0306	0.0489	-3.26	-10.76	1.05
E-N-methylacetamide	0	-10.00	-7.69	-2.31	-0.0318	0.0422	-3.31	-10.99	0.99
Z-N-methylacetamide	0	-10.00	-7.21	-2.79	-0.0318	0.0475	-3.62	-10.83	0.83
benzamide	0	-10.90	-8.44	-2.46	-0.0297	0.0484	-2.94	-11.38	0.48
2,6-dichlorothiobenzamide	0	-10.81	-9.79	-1.02	-0.0193	0.0582	-1.43	-11.22	0.41
urea	0	-13.80	-9.03	-4.77	-0.0298	0.0479	-2.94	-11.97	-1.83
1,1-dimethyl-3-phenylurea	0	-9.63	-8.08	-1.55	-0.0292	0.0443	-2.55	-10.63	1.00
hydrazine	0	-6.26	-4.13	-2.13	-0.0257	0.0317	-1.08	-5.21	-1.05
methylhydrazine	0	-5.31	-3.72	-1.59	-0.0258	0.0311	-1.11	-4.83	-0.48
1,1-dimethylhydrazine	0	-4.48	-3.60	-0.88	-0.0260	0.0309	-1.14	-4.74	0.26
2-methylpyrazine	0	-5.57	-3.71	-1.86	-0.0239	0.0230	-0.52	-4.23	-1.34
2-ethylpyrazine	0	-5.51	-3.43	-2.08	-0.0240	0.0228	-0.53	-3.96	-1.55
morpholine	0	-7.17	-2.50	-4.67	-0.0268	0.0303	-1.33	-3.83	-3.34
N-methylmorpholine	0	-6.34	-3.05	-3.29	-0.0266	0.0142	-1.07	-4.12	-2.22
acetonitrile	0	-3.89	-5.54	1.65	-0.0259	0.0269	-1.03	-6.57	2.68
butanonitrile	0	-3.64	-5.54	1.90	-0.0260	0.0243	-1.02	-6.56	2.92
propionitrile	0	-3.85	-5.05	1.20	-0.0261	0.0246	-1.04	-6.09	2.24
benzonitrile	0	-4.10	-5.96	1.86	-0.0256	0.0266	-0.95	-6.91	2.81

2,6-dichlorobenzonitrile	0	-5.22	-6.26	1.04	-0.0247	0.0296	-0.82	-7.08	1.86
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-7.28	-1.72	-0.0242	0.0555	-2.01	-9.29	0.29
trimethylphosphate	0	-8.70	-7.88	-0.82	-0.0307	0.0234	-2.38	-10.27	1.57
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-7.07	0.46	-0.0273	0.0334	-1.54	-8.61	2.00
phosphine	0	0.60	-0.29	0.89	-0.0108	0.0173	0.98	0.69	-0.09
hydrogen sulfide	0	-0.70	-1.17	0.47	-0.0113	0.0275	0.83	-0.34	-0.36
dimethyl sulfide	0	-1.54	-1.17	-0.37	-0.0158	0.0176	0.67	-0.49	-1.05
diethyl sulfide	0	-1.43	-0.67	-0.76	-0.0165	0.0144	0.64	-0.03	-1.40
dipropyl sulfide	0	-1.27	-2.13	0.86	-0.0166	0.0139	0.62	-1.51	0.24
bis(2-chloroethyl)sulfide	0	-3.92	-4.59	0.67	-0.0117	0.0230	0.89	-3.71	-0.21
dimethyl disulfide	0	-1.83	-0.79	-1.04	-0.0126	0.0199	0.87	0.09	-1.92
diethyl disulfide	0	-1.63	-2.34	0.71	-0.0131	0.0180	0.86	-1.47	-0.16
methanethiol	0	-1.24	-1.21	-0.03	-0.0140	0.0233	0.75	-0.46	-0.78
ethanethiol	0	-1.30	-1.02	-0.28	-0.0143	0.0224	0.74	-0.27	-1.03
1-propanethiol	0	-1.05	-2.10	1.05	-0.0144	0.0223	0.74	-1.36	0.31
thiophene	0	-1.42	-1.23	-0.19	-0.0081	0.0249	0.97	-0.26	-1.16
thiophenol	0	-2.55	-3.39	0.84	-0.0112	0.0271	0.84	-2.55	0.00
thioanisole	0	-2.73	-3.53	0.80	-0.0133	0.0204	0.83	-2.69	-0.04
tetramethylsilane	0	3.04	-0.72	3.76	-0.0047	0.0115	1.14	0.41	2.63
acetylene	-1	-76.50	-62.30	-14.20	-0.0473	0.0081	-11.93	-74.24	-2.26
acetonitrile	-1	-66.60	-57.54	-9.06	-0.0470	-0.0051	-11.68	-69.22	2.62
cyanamide	-1	-72.20	-60.85	-11.35	-0.0473	0.0091	-11.93	-72.78	0.58
aniline	-1	-62.90	-52.83	-10.07	-0.0482	0.0043	-12.73	-65.56	2.66
diphenylamine	-1	-54.60	-46.48	-8.12	-0.0421	0.0073	-7.99	-54.47	-0.13
hydrogen cyanide	-1	-70.20	-63.11	-7.09	-0.0471	-0.0339	-11.79	-74.90	4.70
formic acid	-1	-76.20	-63.61	-12.59	-0.0489	-0.0083	-13.42	-77.03	0.83
acetic acid	-1	-77.60	-62.64	-14.96	-0.0500	0.0008	-14.36	-77.00	-0.60
propanoic acid	-1	-76.20	-60.78	-15.42	-0.0499	0.0026	-14.33	-75.11	-1.09
hexanoic acid	-1	-74.60	-59.95	-14.65	-0.0500	0.0088	-14.39	-74.34	-0.26
acrylic acid	-1	-74.00	-61.37	-12.63	-0.0496	0.0094	-14.07	-75.43	1.43
pyruvic acid	-1	-68.50	-60.25	-8.25	-0.0471	0.0123	-11.80	-72.05	3.55
benzoic acid	-1	-71.20	-58.70	-12.50	-0.0490	0.0128	-13.52	-72.21	1.01
methanol	-1	-95.00	-65.40	-29.60	-0.0595	-0.0187	-25.55	-90.95	-4.05
ethanol	-1	-90.70	-62.34	-28.36	-0.0593	-0.0041	-25.32	-87.66	-3.04
1-propanol	-1	-88.30	-61.45	-26.85	-0.0595	0.0013	-25.48	-86.94	-1.36

isopropanol	-1	-86.30	-59.63	-26.67	-0.0592	-0.0038	-25.07	-84.70	-1.60
2-butanol	-1	-84.20	-56.82	-27.38	-0.0582	-0.0035	-23.80	-80.62	-3.58
t-butanol	-1	-82.30	-57.26	-25.04	-0.0590	-0.0033	-24.84	-82.09	-0.21
allyl alcohol	-1	-86.60	-61.14	-25.46	-0.0587	0.0030	-24.46	-85.60	-1.00
benzyl alcohol	-1	-85.10	-57.39	-27.71	-0.0573	0.0095	-22.66	-80.05	-5.05
2-methoxyethanol	-1	-89.40	-62.47	-26.93	-0.0589	0.0064	-24.67	-87.14	-2.26
phenol	-1	-71.90	-55.32	-16.58	-0.0517	0.0050	-16.13	-71.44	-0.46
2-methylphenol	-1	-70.20	-53.46	-16.74	-0.0516	0.0040	-15.99	-69.46	-0.74
3-methylphenol	-1	-71.10	-55.12	-15.98	-0.0519	0.0059	-16.34	-71.45	0.35
4-methylphenol	-1	-72.00	-55.13	-16.87	-0.0524	0.0046	-16.86	-71.99	-0.01
1,2-ethanediol	-1	-85.30	-64.77	-20.53	-0.0590	0.0407	-25.46	-90.23	4.93
3-hydroxyphenol	-1	-73.80	-56.41	-17.39	-0.0507	0.0483	-16.05	-72.46	-1.34
4-hydroxyphenol	-1	-77.60	-58.05	-19.55	-0.0525	0.0456	-17.83	-75.88	-1.72
methyl hydroperoxide	-1	-93.20	-67.12	-26.08	-0.0567	-0.0034	-21.81	-88.93	-4.27
ethyl hydroperoxide	-1	-89.20	-66.01	-23.19	-0.0568	0.0031	-21.98	-87.99	-1.21
acetaldehyde	-1	-76.50	-60.02	-16.48	-0.0529	-0.0059	-17.38	-77.40	0.90
acetone	-1	-76.20	-58.61	-17.59	-0.0532	-0.0009	-17.69	-76.30	0.10
3-pentanone	-1	-73.70	-53.91	-19.79	-0.0526	0.0006	-17.08	-70.99	-2.71
water	-1	-104.70	-74.20	-30.50	-0.0620	-0.0093	-29.22	-103.42	-1.28
hydrogen peroxide	-1	-97.30	-71.91	-25.39	-0.0569	0.0207	-22.20	-94.11	-3.19
hydroperoxyl radical	-1	-83.30	-69.40	-13.90	-0.0513	-0.0438	-15.67	-85.07	1.77
2-nitrophenol	-1	-60.10	-53.35	-6.75	-0.0462	0.0124	-11.05	-64.40	4.30
3-nitrophenol	-1	-61.90	-50.19	-11.71	-0.0483	0.0174	-12.88	-63.07	1.17
4-nitrophenol	-1	-57.80	-48.61	-9.19	-0.0442	0.0132	-9.50	-58.11	0.31
nitromethane	-1	-76.50	-61.28	-15.22	-0.0481	0.0042	-12.61	-73.89	-2.61
4-nitroaniline	-1	-57.40	-47.82	-9.58	-0.0410	0.0122	-7.27	-55.09	-2.31
acetamide	-1	-80.20	-59.71	-20.49	-0.0505	-0.0007	-14.86	-74.57	-5.63
methanethiol	-1	-73.80	-57.99	-15.81	-0.0388	-0.0045	-5.93	-63.92	-9.88
ethanethiol	-1	-71.80	-56.03	-15.77	-0.0388	-0.0004	-5.94	-61.97	-9.83
1-propanethiol	-1	-70.50	-55.61	-14.89	-0.0389	0.0044	-5.98	-61.59	-8.91
thiophenol	-1	-63.40	-52.44	-10.96	-0.0357	0.0089	-4.32	-56.75	-6.65
hydrogen sulfide	-1	-72.10	-59.62	-12.48	-0.0381	-0.0096	-5.52	-65.14	-6.96
dimethyl sulfoxide	-1	-67.70	-56.69	-11.01	-0.0500	0.0044	-14.41	-71.10	3.40
hydrofluoric acid	-1	-104.40	-80.77	-23.63	-0.0661	-0.0661	-35.82	-116.59	12.19
hydrochloric acid	-1	-74.50	-63.83	-10.67	-0.0402	-0.0402	-6.77	-70.61	-3.89

hydrobromic acid	-1	-68.30	-59.99	-8.31	-0.0352	-0.0352	-4.09	-64.08	-4.22
chloroform	-1	-54.10	-49.18	-4.92	-0.0337	-0.0105	-3.43	-52.61	-1.49
trifluoroacetic acid	-1	-59.30	-56.05	-3.25	-0.0443	0.0226	-9.63	-65.68	6.38
chloroacetic acid	-1	-69.70	-57.87	-11.83	-0.0466	0.0100	-11.38	-69.25	-0.45
dichloroacetic acid	-1	-62.30	-54.63	-7.67	-0.0444	0.0159	-9.68	-64.31	2.01
2,2,2-trifluoroethanol	-1	-77.50	-58.75	-18.75	-0.0555	0.0035	-20.38	-79.13	1.63
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-54.06	-11.44	-0.0517	0.0100	-16.08	-70.14	4.64
2-chlorophenol	-1	-66.10	-53.06	-13.04	-0.0496	0.0094	-14.03	-67.09	0.99
4-chlorophenol	-1	-66.00	-51.52	-14.48	-0.0501	0.0094	-14.47	-65.99	-0.01
methylamine	1	-76.40	-69.94	-6.46	0.0239	0.0870	-5.00	-74.94	-1.46
n-propylamine	1	-71.50	-64.90	-6.60	0.0057	0.0857	-4.71	-69.60	-1.90
isopropylamine	1	-69.60	-63.13	-6.47	0.0100	0.0833	-4.23	-67.35	-2.25
tert-butylamine	1	-67.30	-60.38	-6.92	0.0099	0.0814	-3.84	-64.22	-3.08
cyclohexanamine	1	-68.70	-60.27	-8.43	0.0060	0.0826	-4.08	-64.35	-4.35
allylamine	1	-72.00	-65.00	-7.00	-0.0018	0.0868	-4.96	-69.96	-2.04
dimethylamine	1	-68.60	-62.64	-5.96	0.0216	0.0819	-3.94	-66.58	-2.02
diethylamine	1	-63.40	-56.67	-6.73	0.0097	0.0760	-2.88	-59.56	-3.84
di-n-propylamine	1	-60.50	-54.44	-6.06	0.0062	0.0759	-2.87	-57.31	-3.19
diallylamine	1	-61.60	-54.86	-6.74	-0.0009	0.0774	-3.12	-57.98	-3.62
trimethylamine	1	-61.10	-56.57	-4.53	0.0207	0.0778	-3.19	-59.76	-1.34
triethylamine	1	-54.60	-49.27	-5.33	0.0087	0.0664	-1.51	-50.78	-3.82
aniline	1	-72.40	-64.29	-8.11	-0.0001	0.0890	-5.44	-69.73	-2.67
2-methylaniline	1	-70.30	-61.89	-8.41	-0.0011	0.0867	-4.93	-66.82	-3.48
3-methylaniline	1	-69.60	-62.70	-6.90	-0.0012	0.0878	-5.17	-67.87	-1.73
4-methylaniline	1	-69.80	-62.53	-7.27	-0.0006	0.0873	-5.07	-67.59	-2.21
3-aminoaniline	1	-65.80	-64.17	-1.63	-0.0113	0.0876	-5.28	-69.45	3.65
N-methylaniline	1	-62.60	-57.38	-5.22	-0.0010	0.0827	-4.11	-61.49	-1.11
N-ethylaniline	1	-62.20	-54.56	-7.64	-0.0013	0.0796	-3.51	-58.07	-4.13
N,N-dimethylaniline	1	-57.20	-51.72	-5.48	-0.0011	0.0760	-2.90	-54.61	-2.59
4-methyl-N,N-dimethylaniline	1	-55.90	-50.32	-5.58	-0.0013	0.0754	-2.79	-53.11	-2.79
N,N-diethylaniline	1	-54.00	-47.60	-6.40	-0.0024	0.0695	-1.90	-49.51	-4.49
1-aminonaphthalene	1	-67.40	-60.99	-6.41	-0.0019	0.0894	-5.54	-66.53	-0.87
aziridine	1	-70.90	-64.10	-6.80	0.0236	0.0855	-4.68	-68.79	-2.11
azetidine	1	-67.70	-60.65	-7.05	0.0156	0.0798	-3.55	-64.20	-3.50
pyrrolidine	1	-66.00	-58.55	-7.45	0.0108	0.0790	-3.40	-61.95	-4.05

piperidine	1	-64.20	-56.77	-7.43	0.0105	0.0797	-3.53	-60.30	-3.90
azacycloheptane	1	-63.30	-55.19	-8.11	0.0087	0.0797	-3.53	-58.72	-4.58
pyrrole	1	-61.40	-57.09	-4.31	0.0109	0.0830	-4.15	-61.25	-0.15
pyridine	1	-61.10	-55.52	-5.58	0.0124	0.0855	-4.68	-60.20	-0.90
quinoline	1	-56.00	-50.17	-5.83	0.0026	0.0791	-3.42	-53.59	-2.41
piperazine	1	-66.00	-58.45	-7.55	-0.0140	0.0800	-3.88	-62.34	-3.66
acetonitrile	1	-75.30	-64.73	-10.57	0.0277	0.1274	-18.92	-83.65	8.35
ammonia	1	-85.20	-79.20	-6.00	0.0539	0.0937	-6.59	-85.80	0.60
hydrazine	1	-84.60	-76.29	-8.31	-0.0037	0.0916	-6.06	-82.36	-2.24
methanol	1	-93.00	-75.62	-17.38	0.0150	0.1282	-19.31	-94.93	1.93
ethanol	1	-88.40	-70.28	-18.12	0.0122	0.1243	-17.42	-87.70	-0.70
dimethyl ether	1	-79.70	-64.06	-15.64	0.0117	0.1183	-14.78	-78.84	-0.86
diethyl ether	1	-71.50	-56.48	-15.02	0.0077	0.1054	-9.99	-66.47	-5.03
acetone	1	-77.10	-61.47	-15.63	0.0058	0.1079	-10.83	-72.31	-4.79
acetophenone	1	-64.50	-51.02	-13.48	0.0021	0.0919	-6.13	-57.15	-7.35
water	1	-110.30	-91.73	-18.57	0.0203	0.1431	-27.62	-119.35	9.05
4-methoxyaniline	1	-71.20	-63.18	-8.02	-0.0158	0.0880	-5.66	-68.84	-2.36
4-nitroaniline	1	-75.90	-76.10	0.20	-0.0152	0.0947	-7.24	-83.34	7.44
morpholine	1	-69.60	-62.32	-7.28	-0.0140	0.0826	-4.38	-66.70	-2.90
acetamide	1	-73.90	-65.74	-8.16	0.0014	0.1027	-9.14	-74.88	0.98
benzamide	1	-67.20	-58.23	-8.97	0.0010	0.0997	-8.23	-66.46	-0.74
dimethyl sulfide	1	-64.50	-57.84	-6.66	0.0170	0.0615	-0.94	-58.78	-5.72
dimethyl sulfoxide	1	-67.70	-58.83	-8.87	-0.0019	0.0985	-7.88	-66.71	-0.99
3-chloroaniline	1	-74.70	-66.97	-7.73	-0.0042	0.0916	-6.07	-73.04	-1.66
4-chloroaniline	1	-74.10	-67.28	-6.82	-0.0027	0.0913	-6.00	-73.28	-0.82
PEARSON			0.99					1.00	

Table S 5-2

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/G3large method for the cavity surface with constant density = 0.001 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.16	2.16	-0.0008	0.0198	2.09	1.93	0.07
ethane	0	1.83	0.04	1.79	-0.0013	0.0175	2.09	2.13	-0.30
n-propane	0	1.96	0.13	1.83	-0.0015	0.0171	2.09	2.22	-0.26
n-butane	0	2.08	0.22	1.86	-0.0016	0.0173	2.09	2.31	-0.23
n-pentane	0	2.33	0.32	2.01	-0.0017	0.0171	2.09	2.41	-0.08
n-hexane	0	2.49	0.42	2.07	-0.0017	0.0172	2.09	2.51	-0.02
n-heptane	0	2.62	-0.61	3.23	-0.0018	0.0168	2.09	1.48	1.14
n-octane	0	2.89	-0.66	3.55	-0.0019	0.0167	2.09	1.43	1.46
2-methylpropane	0	2.32	0.13	2.19	-0.0016	0.0172	2.09	2.22	0.10
2,2-dimethylpropane	0	2.50	0.12	2.38	-0.0015	0.0172	2.09	2.21	0.29
2-methylpentane	0	2.52	-0.58	3.10	-0.0020	0.0172	2.09	1.51	1.01
2,4-dimethylpentane	0	2.88	-0.72	3.60	-0.0019	0.0177	2.09	1.38	1.50
2,2,4-trimethylpentane	0	2.85	-0.84	3.69	-0.0023	0.0184	2.09	1.25	1.60
cyclopropane	0	0.75	-0.63	1.38	-0.0094	0.0218	2.07	1.43	-0.68
cyclopentane	0	1.20	0.40	0.80	-0.0021	0.0166	2.09	2.49	-1.29
cyclohexane	0	1.23	-0.39	1.62	-0.0019	0.0156	2.09	1.70	-0.47
methylcyclohexane	0	1.71	-0.50	2.21	-0.0019	0.0169	2.09	1.59	0.12
cis-1,2-dimethylcyclohexane	0	1.58	-0.59	2.17	-0.0020	0.0176	2.09	1.50	0.08
ethene	0	1.27	-1.15	2.42	-0.0125	0.0266	2.03	0.88	0.39
propene	0	1.27	-0.97	2.24	-0.0134	0.0246	2.02	1.04	0.23
1-butene	0	1.38	-0.78	2.16	-0.0137	0.0240	2.01	1.23	0.15
1-pentene	0	1.66	-0.70	2.36	-0.0138	0.0238	2.01	1.31	0.35
E-2-pentene	0	1.34	-0.53	1.87	-0.0137	0.0223	2.02	1.48	-0.14
1-hexene	0	1.68	-0.67	2.35	-0.0137	0.0239	2.01	1.34	0.34
2-methylpropene	0	1.16	-0.86	2.02	-0.0142	0.0223	2.01	1.14	0.02
s-trans-1,3-butadiene	0	0.61	-1.85	2.46	-0.0109	0.0272	2.05	0.20	0.41
cyclopentene	0	0.56	-0.38	0.94	-0.0141	0.0252	2.00	1.63	-1.07
ethyne	0	-0.01	-4.05	4.04	-0.0131	0.0573	1.80	-2.25	2.24
propyne	0	-0.31	-3.17	2.86	-0.0154	0.0519	1.82	-1.35	1.04
1-butyne	0	-0.16	-2.91	2.75	-0.0158	0.0518	1.81	-1.09	0.93
1-pentyne	0	0.01	-2.63	2.64	-0.0159	0.0513	1.82	-0.81	0.82
1-hexyne	0	0.29	-2.73	3.02	-0.0160	0.0509	1.82	-0.91	1.20

butenyne	0	0.04	-3.50	3.54	-0.0150	0.0541	1.81	-1.69	1.73
benzene	0	-0.87	-2.16	1.29	-0.0065	0.0279	2.07	-0.09	-0.78
ethylbenzene	0	-0.80	-3.04	2.24	-0.0076	0.0272	2.07	-0.97	0.17
naphthalene	0	-2.39	-4.40	2.01	-0.0072	0.0283	2.07	-2.33	-0.06
anthracene	0	-4.23	-5.67	1.44	-0.0076	0.0287	2.07	-3.60	-0.63
toluene	0	-0.89	-3.00	2.11	-0.0076	0.0273	2.07	-0.93	0.04
p-xylene	0	-0.81	-2.88	2.07	-0.0085	0.0253	2.07	-0.81	0.00
m-xylene	0	-0.84	-2.92	2.08	-0.0087	0.0267	2.07	-0.85	0.01
o-xylene	0	-0.90	-3.02	2.12	-0.0085	0.0262	2.07	-0.95	0.05
fluoromethane	0	-0.22	-2.30	2.08	-0.0218	0.0288	1.70	-0.61	0.39
chloromethane	0	-0.56	-1.33	0.77	-0.0110	0.0328	2.03	0.70	-1.26
bromomethane	0	-0.82	-1.42	0.60	-0.0089	0.0340	2.04	0.62	-1.44
chlorofluoromethane	0	-0.77	-1.96	1.19	-0.0140	0.0428	1.94	-0.02	-0.75
dichloromethane	0	-1.36	-0.83	-0.53	-0.0062	0.0441	2.00	1.17	-2.53
dibromomethane	0	-2.11	-1.02	-1.09	-0.0046	0.0448	2.00	0.98	-3.09
chlorodifluoromethane	0	-0.50	-0.65	0.15	-0.0081	0.0540	1.90	1.24	-1.74
chloroform	0	-1.07	1.22	-2.29	-0.0025	0.0528	1.92	3.14	-4.21
chloroethane	0	-0.63	-1.16	0.53	-0.0121	0.0310	2.02	0.86	-1.49
bromoethane	0	-0.70	-1.29	0.59	-0.0099	0.0322	2.04	0.75	-1.45
bromoform	0	-1.98	-3.66	1.68	-0.0015	0.0525	1.92	-1.74	-0.24
tetrafluoromethane	0	3.16	2.41	0.75	-0.0019	0.0541	1.90	4.32	-1.16
difluorodichloromethane	0	1.69	3.53	-1.84	-0.0035	0.0369	2.05	5.58	-3.89
fluorotrichloromethane	0	0.82	3.98	-3.16	-0.0043	0.0363	2.05	6.03	-5.21
bromotrifluoromethane	0	1.79	2.68	-0.89	-0.0030	0.0528	1.92	4.60	-2.81
bromotrichloromethane	0	-0.93	-1.85	0.92	0.0000	0.0409	2.02	0.17	-1.10
hexafluoroethane	0	3.94	-1.60	5.54	-0.0021	0.0545	1.90	0.30	3.64
hexachloroethane	0	-1.40	-2.26	0.86	-0.0016	0.0342	2.06	-0.20	-1.20
chloropentafluoroethane	0	2.86	-1.58	4.44	-0.0031	0.0515	1.93	0.36	2.50
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.84	3.61	-0.0054	0.0368	2.04	0.21	1.56
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-4.55	5.07	-0.0089	0.0555	1.87	-2.68	3.20
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-4.14	4.01	-0.0056	0.0546	1.90	-2.24	2.11
1-chloro-2,2,2-trifluoroethane	0	0.06	-0.38	0.44	-0.0075	0.0456	1.98	1.61	-1.55
1,1,1,2-tetrachloroethane	0	-1.15	-3.95	2.80	-0.0062	0.0434	2.00	-1.95	0.80
1,1,1-trichloroethane	0	-0.25	-2.71	2.46	-0.0044	0.0325	2.06	-0.64	0.39
1,1,2-trichloroethane	0	-1.95	-4.85	2.90	-0.0076	0.0464	1.98	-2.88	0.93

1,1-difluoroethane	0	-0.11	-2.43	2.32	-0.0167	0.0379	1.90	-0.53	0.42
1-bromo-2-chloroethane	0	-1.95	-1.02	-0.93	-0.0087	0.0370	2.03	1.01	-2.96
octafluoropropane	0	4.28	-1.88	6.16	-0.0021	0.0537	1.91	0.03	4.25
2-chloropropane	0	-0.25	-1.04	0.79	-0.0129	0.0297	2.02	0.97	-1.22
1-chloropropane	0	-0.27	-0.99	0.72	-0.0121	0.0303	2.02	1.03	-1.30
1-bromopropane	0	-0.56	-3.02	2.46	-0.0100	0.0315	2.04	-0.97	0.41
2-bromopropane	0	-0.48	-3.01	2.53	-0.0107	0.0311	2.04	-0.98	0.50
2-chlorobutane	0	0.07	-2.83	2.90	-0.0130	0.0290	2.02	-0.82	0.89
1-bromobutane	0	-0.41	-1.06	0.65	-0.0101	0.0313	2.04	0.98	-1.39
1-chloropentane	0	0.07	-3.13	3.20	-0.0123	0.0301	2.02	-1.11	1.18
2-chloropentane	0	0.07	-2.87	2.94	-0.0130	0.0289	2.02	-0.86	0.93
1-bromopentane	0	-0.08	-3.14	3.06	-0.0102	0.0314	2.04	-1.10	1.02
1-bromo-isobutane	0	-0.03	-2.89	2.86	-0.0101	0.0315	2.04	-0.85	0.82
tetrachloroethene	0	0.05	4.48	-4.43	-0.0022	0.0331	2.06	6.54	-6.49
trichloroethene	0	-0.39	2.18	-2.57	-0.0035	0.0478	1.97	4.16	-4.55
chloroethene	0	-0.59	-0.83	0.24	-0.0088	0.0385	2.02	1.19	-1.78
E-1,2-dichloroethene	0	-0.76	0.40	-1.16	-0.0060	0.0438	2.00	2.40	-3.16
Z-1,2-dichloroethene	0	-1.17	-0.37	-0.80	-0.0055	0.0444	2.00	1.63	-2.80
3-chloropropene	0	-0.57	-1.60	1.03	-0.0107	0.0335	2.03	0.43	-1.00
3-bromopropene	0	-0.86	-2.09	1.23	-0.0095	0.0350	2.04	-0.05	-0.81
fluorobenzene	0	-0.78	-3.68	2.90	-0.0166	0.0329	1.92	-1.76	0.98
chlorobenzene	0	-1.12	-1.02	-0.10	-0.0084	0.0326	2.05	1.03	-2.15
bromobenzene	0	-1.46	-3.47	2.01	-0.0068	0.0331	2.06	-1.42	-0.04
1,4-dichlorobenzene	0	-1.01	-3.51	2.50	-0.0068	0.0361	2.04	-1.46	0.45
1,2-dichlorobenzene	0	-1.36	0.13	-1.49	-0.0075	0.0358	2.04	2.17	-3.53
p-dibromobenzene	0	-2.30	-3.67	1.37	-0.0055	0.0362	2.05	-1.62	-0.68
chlorotoluene	0	-1.92	-5.46	3.54	-0.0120	0.0336	2.02	-3.45	1.53
o-chlorotoluene	0	-1.15	-3.16	2.01	-0.0090	0.0324	2.05	-1.11	-0.04
bromotoluene	0	-2.37	-5.48	3.11	-0.0100	0.0351	2.03	-3.45	1.08
p-bromotoluene	0	-1.39	-3.47	2.08	-0.0072	0.0326	2.06	-1.41	0.02
2,3-dichlorobiphenyl	0	-2.45	-5.36	2.91	-0.0077	0.0349	2.05	-3.32	0.87
2,2'-dichlorobiphenyl	0	-2.73	-5.77	3.04	-0.0091	0.0326	2.05	-3.72	0.99
2,2',3'-trichlorobiphenyl	0	-1.99	-5.65	3.66	-0.0089	0.0354	2.04	-3.62	1.63
1,2-dimethoxyethane	0	-4.84	-3.29	-1.55	-0.0296	0.0225	0.95	-2.34	-2.50
anisole	0	-2.45	-4.76	2.31	-0.0262	0.0296	1.34	-3.43	0.98

dimethyl ether	0	-1.92	-2.41	0.49	-0.0308	0.0227	0.77	-1.63	-0.29
diethyl ether	0	-1.76	-2.23	0.47	-0.0320	0.0211	0.58	-1.65	-0.11
isopropyl ether	0	-0.53	-3.09	2.56	-0.0323	0.0215	0.53	-2.56	2.03
methyl propyl ether	0	-1.66	-1.98	0.32	-0.0307	0.0219	0.79	-1.19	-0.47
methyl isopropyl ether	0	-2.01	-3.00	0.99	-0.0311	0.0215	0.73	-2.27	0.26
t-butyl methyl ether	0	-2.21	-3.00	0.79	-0.0313	0.0211	0.70	-2.29	0.08
ethyl phenyl ether	0	-2.22	-4.63	2.41	-0.0263	0.0294	1.33	-3.30	1.08
tetrahydrofuran	0	-3.47	-2.44	-1.03	-0.0326	0.0220	0.48	-1.96	-1.51
tetrahydropyran	0	-3.12	-3.22	0.10	-0.0322	0.0204	0.55	-2.67	-0.45
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-5.61	5.49	-0.0190	0.0436	1.78	-3.83	3.71
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-6.83	6.94	-0.0122	0.0552	1.84	-4.99	5.10
acetaldehyde	0	-3.50	-5.96	2.46	-0.0317	0.0383	0.59	-5.36	1.86
propanal	0	-3.44	-5.38	1.94	-0.0319	0.0366	0.55	-4.82	1.38
butanal	0	-3.18	-5.44	2.26	-0.0317	0.0355	0.59	-4.85	1.67
pentanal	0	-3.03	-6.33	3.30	-0.0322	0.0355	0.52	-5.81	2.78
octanal	0	-2.29	-6.49	4.20	-0.0321	0.0358	0.53	-5.95	3.66
benzaldehyde	0	-4.02	-7.60	3.58	-0.0323	0.0348	0.50	-7.10	3.08
p-hydroxybenzaldehyde	0	-10.48	-12.70	2.22	-0.0335	0.0928	-1.00	-13.70	3.22
m-hydroxybenzaldehyde	0	-9.51	-12.18	2.67	-0.0318	0.0928	-0.70	-12.88	3.37
acetone	0	-3.85	-5.93	2.08	-0.0332	0.0335	0.34	-5.59	1.74
2-butanone	0	-3.64	-5.35	1.71	-0.0335	0.0325	0.28	-5.07	1.43
2-pentanone	0	-3.53	-6.36	2.83	-0.0336	0.0323	0.27	-6.09	2.56
3-pentanone	0	-3.41	-5.88	2.47	-0.0327	0.0321	0.44	-5.44	2.03
2-hexanone	0	-3.29	-6.44	3.15	-0.0336	0.0321	0.28	-6.16	2.87
2-heptanone	0	-3.04	-6.49	3.45	-0.0337	0.0323	0.25	-6.24	3.20
4-heptanone	0	-2.93	-5.96	3.03	-0.0328	0.0318	0.42	-5.54	2.61
2-octanone	0	-2.88	-6.56	3.68	-0.0336	0.0289	0.29	-6.28	3.40
5-nonanone	0	-2.67	-6.09	3.42	-0.0329	0.0313	0.40	-5.69	3.02
3,3-dimethylbutanone	0	-2.89	-6.08	3.19	-0.0338	0.0289	0.25	-5.82	2.93
cyclopentanone	0	-4.68	-6.89	2.21	-0.0334	0.0335	0.31	-6.58	1.90
acetophenone	0	-4.58	-7.52	2.94	-0.0337	0.0328	0.25	-7.28	2.70
methyl formate	0	-2.78	-5.44	2.66	-0.0295	0.0433	0.88	-4.56	1.78
ethyl formate	0	-2.65	-5.23	2.58	-0.0300	0.0430	0.82	-4.42	1.77
methyl acetate	0	-3.32	-5.00	1.68	-0.0315	0.0381	0.63	-4.37	1.05
ethyl acetate	0	-3.10	-6.14	3.04	-0.0318	0.0370	0.58	-5.56	2.46

propyl acetate	0	-2.86	-6.18	3.32	-0.0319	0.0355	0.57	-5.61	2.75
butyl acetate	0	-2.55	-6.23	3.68	-0.0320	0.0368	0.55	-5.68	3.13
methyl propanoate	0	-2.93	-4.52	1.59	-0.0310	0.0371	0.70	-3.82	0.89
methyl butanoate	0	-2.83	-5.91	3.08	-0.0310	0.0371	0.70	-5.21	2.38
methyl pentanoate	0	-2.57	-5.98	3.41	-0.0312	0.0365	0.67	-5.32	2.75
methyl hexanoate	0	-2.49	-6.06	3.57	-0.0311	0.0362	0.69	-5.36	2.87
methyl benzoate	0	-3.91	-6.63	2.72	-0.0314	0.0347	0.65	-5.98	2.07
hydrogen	0	2.33	-0.27	2.60	-0.0011	0.0230	2.09	1.82	0.51
water	0	-6.31	-7.71	1.40	-0.0305	0.0826	-0.05	-7.76	1.45
water dimer	0	-11.27	-12.18	0.91	-0.0345	0.0897	-1.05	-13.23	1.96
hydrogen peroxide	0	-8.58	-8.66	0.08	-0.0252	0.0942	0.07	-8.60	0.02
methyl peroxide	0	-5.28	-6.09	0.81	-0.0261	0.0923	0.08	-6.01	0.73
ethyl peroxide	0	-5.32	-5.93	0.61	-0.0265	0.0907	0.11	-5.81	0.49
1,4-dioxane	0	-5.05	-4.06	-0.99	-0.0302	0.0253	0.86	-3.20	-1.85
methanol	0	-5.11	-5.17	0.06	-0.0309	0.0783	0.05	-5.12	0.01
ethanol	0	-5.01	-4.76	-0.25	-0.0309	0.0770	0.09	-4.67	-0.34
1-propanol	0	-4.83	-4.63	-0.20	-0.0310	0.0755	0.13	-4.50	-0.33
isopropanol	0	-4.76	-4.60	-0.16	-0.0318	0.0730	0.07	-4.52	-0.24
1-butanol	0	-4.72	-4.53	-0.19	-0.0311	0.0750	0.12	-4.41	-0.31
t-butanol	0	-4.51	-4.31	-0.20	-0.0315	0.0716	0.15	-4.16	-0.35
1-pentanol	0	-4.47	-5.80	1.33	-0.0316	0.0738	0.07	-5.73	1.26
1-hexanol	0	-4.36	-5.89	1.53	-0.0317	0.0754	0.01	-5.88	1.52
1-heptanol	0	-4.24	-5.99	1.75	-0.0317	0.0725	0.09	-5.90	1.66
1-octanol	0	-4.09	-6.44	2.35	-0.0318	0.0744	0.03	-6.41	2.32
allyl alcohol	0	-5.08	-5.03	-0.05	-0.0307	0.0775	0.10	-4.92	-0.16
cyclopentanol	0	-5.49	-5.17	-0.32	-0.0318	0.0695	0.17	-5.00	-0.49
2-methoxyethanol	0	-6.77	-6.53	-0.24	-0.0303	0.0796	0.10	-6.42	-0.35
2,2,2-trifluoroethanol	0	-4.31	-9.26	4.95	-0.0237	0.0905	0.38	-8.88	4.57
1,1,1-trifluoropropan-2-ol	0	-4.16	-6.62	2.46	-0.0263	0.0839	0.43	-6.18	2.02
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-7.71	3.94	-0.0203	0.0963	0.29	-7.41	3.64
phenol	0	-6.62	-6.41	-0.21	-0.0252	0.0879	0.37	-6.04	-0.58
p-bromophenol	0	-7.13	-8.29	1.16	-0.0234	0.0886	0.49	-7.80	0.67
o-cresol	0	-5.87	-7.16	1.29	-0.0248	0.0863	0.48	-6.69	0.82
m-cresol	0	-5.49	-7.58	2.09	-0.0256	0.0887	0.31	-7.28	1.79
p-cresol	0	-6.14	-7.52	1.38	-0.0258	0.0878	0.32	-7.20	1.06

1,2-ethanediol	0	-9.30	-8.21	-1.09	-0.0325	0.0835	-0.40	-8.61	-0.69
acetic acid	0	-6.70	-7.76	1.06	-0.0306	0.0974	-0.75	-8.51	1.81
propanoic acid	0	-6.47	-7.27	0.80	-0.0300	0.0969	-0.65	-7.91	1.44
butanoic acid	0	-6.36	-7.13	0.77	-0.0301	0.0964	-0.63	-7.76	1.40
pentanoic acid	0	-6.16	-8.60	2.44	-0.0301	0.0969	-0.65	-9.25	3.09
hexanoic acid	0	-6.21	-8.65	2.44	-0.0302	0.0968	-0.66	-9.31	3.10
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-14.10	2.14	-0.0266	0.1002	-0.42	-14.52	2.56
ammonia	0	-4.29	-4.61	0.32	-0.0337	0.0463	0.16	-4.44	0.15
methylamine	0	-4.56	-3.52	-1.04	-0.0336	0.0437	0.21	-3.31	-1.25
ethylamine	0	-4.50	-3.46	-1.04	-0.0339	0.0424	0.16	-3.30	-1.20
butylamine	0	-4.29	-4.21	-0.08	-0.0339	0.0421	0.16	-4.05	-0.24
propylamine	0	-4.39	-3.37	-1.02	-0.0339	0.0428	0.16	-3.21	-1.18
pentylamine	0	-4.10	-4.26	0.16	-0.0341	0.0413	0.14	-4.13	0.03
dimethylamine	0	-4.29	-2.39	-1.90	-0.0325	0.0431	0.42	-1.97	-2.32
diethylamine	0	-4.07	-2.08	-1.99	-0.0325	0.0406	0.44	-1.64	-2.43
dipropylamine	0	-3.66	-3.06	-0.60	-0.0323	0.0406	0.47	-2.58	-1.08
trimethylamine	0	-3.23	-1.25	-1.98	-0.0312	0.0199	0.72	-0.53	-2.70
azetidine	0	-5.56	-2.52	-3.04	-0.0339	0.0416	0.17	-2.35	-3.21
pyrrolidine	0	-5.48	-3.54	-1.94	-0.0340	0.0414	0.16	-3.38	-2.10
piperidine	0	-5.11	-2.63	-2.48	-0.0322	0.0419	0.48	-2.15	-2.96
2-methoxyethanamine	0	-6.55	-5.52	-1.03	-0.0328	0.0443	0.35	-5.16	-1.39
1,2-ethanediamine	0	-9.72	-6.92	-2.80	-0.0329	0.0445	0.33	-6.59	-3.13
nitromethane	0	-3.95	-7.56	3.61	-0.0242	0.0434	1.46	-6.10	2.15
nitroethane	0	-3.71	-6.88	3.17	-0.0249	0.0399	1.42	-5.46	1.75
1-nitropropane	0	-3.34	-6.61	3.27	-0.0249	0.0395	1.42	-5.19	1.85
2-nitropropane	0	-3.14	-5.99	2.85	-0.0254	0.0381	1.39	-4.60	1.46
1-nitrobutane	0	-3.08	-8.09	5.01	-0.0250	0.0393	1.41	-6.67	3.59
nitrobenzene	0	-4.12	-7.34	3.22	-0.0241	0.0396	1.49	-5.85	1.73
2-methyl-1-nitrobenzene	0	-3.59	-6.94	3.35	-0.0252	0.0375	1.40	-5.54	1.95
pyridine	0	-4.70	-5.04	0.34	-0.0331	0.0348	0.36	-4.67	-0.03
2-methylpyridine	0	-4.63	-4.67	0.04	-0.0333	0.0334	0.32	-4.35	-0.28
3-methylpyridine	0	-4.77	-5.02	0.25	-0.0336	0.0328	0.28	-4.75	-0.02
4-methylpyridine	0	-4.94	-4.07	-0.87	-0.0340	0.0301	0.21	-3.87	-1.07
4-ethylpyridine	0	-4.74	-5.17	0.43	-0.0340	0.0303	0.20	-4.97	0.23
2,4-dimethylpyridine	0	-4.86	-4.81	-0.05	-0.0342	0.0287	0.16	-4.65	-0.21

2,5-dimethylpyridine	0	-4.72	-4.64	-0.08	-0.0337	0.0319	0.26	-4.38	-0.34
2,6-dimethylpyridine	0	-4.60	-4.32	-0.28	-0.0335	0.0330	0.29	-4.04	-0.56
3,4-dimethylpyridine	0	-5.22	-5.26	0.04	-0.0344	0.0298	0.13	-5.14	-0.08
3,5-dimethylpyridine	0	-4.84	-5.02	0.18	-0.0340	0.0317	0.19	-4.82	-0.02
aniline	0	-5.49	-6.87	1.38	-0.0260	0.0561	1.17	-5.70	0.21
N-methylaniline	0	-4.68	-5.57	0.89	-0.0232	0.0550	1.42	-4.14	-0.54
2-methylaniline	0	-5.56	-6.36	0.80	-0.0265	0.0538	1.15	-5.21	-0.35
3-methylaniline	0	-5.67	-6.74	1.07	-0.0263	0.0550	1.15	-5.59	-0.08
4-methylaniline	0	-5.55	-6.66	1.11	-0.0267	0.0531	1.13	-5.53	-0.02
N-ethylaniline	0	-4.62	-5.45	0.83	-0.0209	0.0556	1.56	-3.89	-0.73
3-aminoaniline	0	-9.92	-10.64	0.72	-0.0261	0.0553	1.16	-9.48	-0.44
N,N-dimethylaniline	0	-3.58	-4.32	0.74	-0.0192	0.0263	1.84	-2.48	-1.10
piperazine	0	-7.40	-4.79	-2.61	-0.0319	0.0427	0.52	-4.27	-3.13
N-methylpiperazine	0	-7.77	-3.92	-3.85	-0.0318	0.0431	0.54	-3.38	-4.39
N,N'-dimethylpiperazine	0	-7.58	-3.02	-4.56	-0.0303	0.0198	0.85	-2.16	-5.42
1-methylthymine	0	-10.40	-14.53	4.13	-0.0338	0.0789	-0.48	-15.01	4.61
9-methyladenine	0	-13.60	-12.12	-1.48	-0.0340	0.0692	-0.24	-12.36	-1.24
acetamide	0	-9.71	-10.07	0.36	-0.0360	0.0696	-0.68	-10.75	1.04
E-N-methylacetamide	0	-10.00	-9.89	-0.11	-0.0374	0.0618	-0.85	-10.73	0.73
Z-N-methylacetamide	0	-10.00	-9.30	-0.70	-0.0376	0.0680	-1.03	-10.33	0.33
benzamide	0	-10.90	-11.27	0.37	-0.0353	0.0700	-0.52	-11.80	0.90
2,6-dichlorothiobenzamide	0	-10.81	-13.12	2.31	-0.0231	0.0823	0.77	-12.35	1.54
urea	0	-13.80	-12.42	-1.38	-0.0353	0.0682	-0.48	-12.90	-0.90
1,1-dimethyl-3-phenylurea	0	-9.63	-10.61	0.98	-0.0342	0.0643	-0.17	-10.78	1.15
hydrazine	0	-6.26	-6.17	-0.09	-0.0318	0.0472	0.51	-5.66	-0.60
methylhydrazine	0	-5.31	-5.45	0.14	-0.0319	0.0465	0.50	-4.96	-0.35
1,1-dimethylhydrazine	0	-4.48	-5.08	0.60	-0.0321	0.0464	0.46	-4.62	0.14
2-methylpyrazine	0	-5.57	-5.13	-0.44	-0.0291	0.0345	0.98	-4.15	-1.42
2-ethylpyrazine	0	-5.51	-4.80	-0.71	-0.0292	0.0342	0.98	-3.82	-1.69
morpholine	0	-7.17	-4.00	-3.17	-0.0317	0.0451	0.54	-3.46	-3.71
N-methylmorpholine	0	-6.34	-4.30	-2.04	-0.0315	0.0225	0.67	-3.63	-2.71
acetonitrile	0	-3.89	-7.07	3.18	-0.0303	0.0386	0.81	-6.26	2.37
butanonitrile	0	-3.64	-6.97	3.33	-0.0303	0.0353	0.82	-6.16	2.52
propionitrile	0	-3.85	-6.51	2.66	-0.0304	0.0356	0.80	-5.71	1.86
benzonitrile	0	-4.10	-7.63	3.53	-0.0297	0.0382	0.89	-6.74	2.64

2,6-dichlorobenzonitrile	0	-5.22	-7.97	2.75	-0.0286	0.0419	1.01	-6.96	1.74
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-10.15	1.15	-0.0282	0.0811	0.32	-9.83	0.83
trimethylphosphate	0	-8.70	-10.39	1.69	-0.0354	0.0428	-0.14	-10.53	1.83
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-9.85	3.24	-0.0315	0.0501	0.52	-9.32	2.71
phosphine	0	0.60	-0.60	1.20	-0.0124	0.0278	2.03	1.43	-0.83
hydrogen sulfide	0	-0.70	-1.95	1.25	-0.0129	0.0415	1.96	0.01	-0.71
dimethyl sulfide	0	-1.54	-1.99	0.45	-0.0190	0.0271	1.85	-0.15	-1.39
diethyl sulfide	0	-1.43	-1.51	0.08	-0.0198	0.0229	1.82	0.30	-1.73
dipropyl sulfide	0	-1.27	-3.02	1.75	-0.0200	0.0224	1.81	-1.21	-0.06
bis(2-chloroethyl)sulfide	0	-3.92	-6.53	2.61	-0.0143	0.0341	1.97	-4.56	0.64
dimethyl disulfide	0	-1.83	-1.79	-0.04	-0.0147	0.0300	1.98	0.19	-2.02
diethyl disulfide	0	-1.63	-3.28	1.65	-0.0154	0.0274	1.97	-1.31	-0.32
methanethiol	0	-1.24	-2.00	0.76	-0.0164	0.0362	1.91	-0.09	-1.15
ethanethiol	0	-1.30	-1.83	0.53	-0.0168	0.0348	1.91	0.08	-1.38
1-propanethiol	0	-1.05	-2.94	1.89	-0.0169	0.0346	1.90	-1.03	-0.02
thiophene	0	-1.42	-2.22	0.80	-0.0085	0.0368	2.03	-0.18	-1.24
thiophenol	0	-2.55	-4.70	2.15	-0.0125	0.0405	1.98	-2.72	0.17
thioanisole	0	-2.73	-4.83	2.10	-0.0155	0.0304	1.96	-2.87	0.14
tetramethylsilane	0	3.04	-1.16	4.20	-0.0036	0.0192	2.09	0.93	2.11
acetylene	-1	-76.50	-67.50	-9.00	-0.0556	0.0219	-8.92	-76.43	-0.07
acetonitrile	-1	-66.60	-61.24	-5.36	-0.0534	0.0025	-7.44	-68.68	2.08
cyanamide	-1	-72.20	-65.12	-7.08	-0.0537	0.0238	-7.59	-72.71	0.51
aniline	-1	-62.90	-56.82	-6.08	-0.0569	0.0134	-9.85	-66.67	3.77
diphenylamine	-1	-54.60	-49.95	-4.65	-0.0505	0.0165	-5.71	-55.66	1.06
hydrogen cyanide	-1	-70.20	-67.30	-2.90	-0.0534	-0.0352	-7.43	-74.72	4.52
formic acid	-1	-76.20	-67.76	-8.44	-0.0555	0.0027	-8.83	-76.59	0.39
acetic acid	-1	-77.60	-67.08	-10.52	-0.0567	0.0091	-9.73	-76.82	-0.78
propanoic acid	-1	-76.20	-65.10	-11.10	-0.0568	0.0084	-9.80	-74.90	-1.30
hexanoic acid	-1	-74.60	-64.37	-10.23	-0.0569	0.0157	-9.85	-74.22	-0.38
acrylic acid	-1	-74.00	-65.75	-8.25	-0.0565	0.0198	-9.57	-75.32	1.32
pyruvic acid	-1	-68.50	-64.88	-3.62	-0.0534	0.0264	-7.45	-72.33	3.83
benzoic acid	-1	-71.20	-63.06	-8.14	-0.0558	0.0231	-9.07	-72.12	0.92
methanol	-1	-95.00	-70.04	-24.96	-0.0670	-0.0160	-19.45	-89.48	-5.52
ethanol	-1	-90.70	-67.11	-23.59	-0.0674	0.0028	-19.92	-87.03	-3.67
1-propanol	-1	-88.30	-66.29	-22.01	-0.0676	0.0084	-20.07	-86.37	-1.93

isopropanol	-1	-86.30	-64.50	-21.80	-0.0672	0.0030	-19.64	-84.15	-2.15
2-butanol	-1	-84.20	-61.29	-22.91	-0.0666	0.0029	-18.95	-80.24	-3.96
t-butanol	-1	-82.30	-62.22	-20.08	-0.0667	0.0034	-19.11	-81.33	-0.97
allyl alcohol	-1	-86.60	-66.04	-20.56	-0.0670	0.0119	-19.44	-85.49	-1.11
benzyl alcohol	-1	-85.10	-61.91	-23.19	-0.0658	0.0191	-18.11	-80.02	-5.08
2-methoxyethanol	-1	-89.40	-67.63	-21.77	-0.0671	0.0148	-19.56	-87.19	-2.21
phenol	-1	-71.90	-59.29	-12.61	-0.0590	0.0142	-11.49	-70.77	-1.13
2-methylphenol	-1	-70.20	-57.39	-12.81	-0.0591	0.0127	-11.65	-69.03	-1.17
3-methylphenol	-1	-71.10	-59.17	-11.93	-0.0593	0.0144	-11.74	-70.91	-0.19
4-methylphenol	-1	-72.00	-59.19	-12.81	-0.0598	0.0131	-12.18	-71.37	-0.63
1,2-ethanediol	-1	-85.30	-70.68	-14.62	-0.0672	0.0655	-20.00	-90.68	5.38
3-hydroxyphenol	-1	-73.80	-61.33	-12.47	-0.0580	0.0756	-11.31	-72.64	-1.16
4-hydroxyphenol	-1	-77.60	-63.29	-14.31	-0.0599	0.0709	-12.81	-76.09	-1.51
methyl hydroperoxide	-1	-93.20	-72.26	-20.94	-0.0660	0.0041	-18.27	-90.53	-2.67
ethyl hydroperoxide	-1	-89.20	-71.30	-17.90	-0.0661	0.0111	-18.45	-89.76	0.56
acetaldehyde	-1	-76.50	-64.08	-12.42	-0.0601	0.0013	-12.50	-76.58	0.08
acetone	-1	-76.20	-62.90	-13.30	-0.0607	0.0067	-12.97	-75.87	-0.33
3-pentanone	-1	-73.70	-57.74	-15.96	-0.0598	0.0077	-12.18	-69.92	-3.78
water	-1	-104.70	-80.92	-23.78	-0.0711	0.0028	-24.58	-105.49	0.79
hydrogen peroxide	-1	-97.30	-77.78	-19.52	-0.0660	0.0433	-18.38	-96.16	-1.14
hydroperoxyl radical	-1	-83.30	-73.78	-9.52	-0.0578	-0.0462	-10.59	-84.37	1.07
2-nitrophenol	-1	-60.10	-57.06	-3.04	-0.0527	0.0240	-6.96	-64.02	3.92
3-nitrophenol	-1	-61.90	-53.84	-8.06	-0.0554	0.0306	-8.75	-62.59	0.69
4-nitrophenol	-1	-57.80	-51.99	-5.81	-0.0509	0.0260	-5.92	-57.90	0.10
nitromethane	-1	-76.50	-65.30	-11.20	-0.0544	0.0151	-8.06	-73.36	-3.14
4-nitroaniline	-1	-57.40	-51.28	-6.12	-0.0483	0.0247	-4.57	-55.84	-1.56
acetamide	-1	-80.20	-64.25	-15.95	-0.0573	0.0086	-10.19	-74.44	-5.76
methanethiol	-1	-73.80	-62.81	-10.99	-0.0454	0.0027	-3.22	-66.03	-7.77
ethanethiol	-1	-71.80	-60.87	-10.93	-0.0456	0.0075	-3.28	-64.14	-7.66
1-propanethiol	-1	-70.50	-60.54	-9.96	-0.0456	0.0118	-3.31	-63.85	-6.65
thiophenol	-1	-63.40	-56.64	-6.76	-0.0417	0.0188	-1.81	-58.45	-4.95
hydrogen sulfide	-1	-72.10	-64.34	-7.76	-0.0439	-0.0015	-2.62	-66.96	-5.14
dimethyl sulfoxide	-1	-67.70	-61.04	-6.66	-0.0571	0.0147	-10.03	-71.06	3.36
hydrofluoric acid	-1	-104.40	-87.14	-17.26	-0.0758	-0.0758	-31.41	-118.55	14.15
hydrochloric acid	-1	-74.50	-68.59	-5.91	-0.0449	-0.0449	-2.98	-71.58	-2.92

hydrobromic acid	-1	-68.30	-64.17	-4.13	-0.0386	-0.0386	-0.85	-65.03	-3.27
chloroform	-1	-54.10	-51.30	-2.80	-0.0391	-0.0050	-1.00	-52.30	-1.80
trifluoroacetic acid	-1	-59.30	-59.27	-0.03	-0.0499	0.0394	-5.43	-64.70	5.40
chloroacetic acid	-1	-69.70	-62.02	-7.68	-0.0530	0.0212	-7.16	-69.18	-0.52
dichloroacetic acid	-1	-62.30	-58.24	-4.06	-0.0503	0.0292	-5.62	-63.86	1.56
2,2,2-trifluoroethanol	-1	-77.50	-62.55	-14.95	-0.0632	0.0153	-15.30	-77.85	0.35
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-57.37	-8.13	-0.0588	0.0238	-11.36	-68.73	3.23
2-chlorophenol	-1	-66.10	-56.67	-9.43	-0.0567	0.0199	-9.74	-66.40	0.30
4-chlorophenol	-1	-66.00	-55.07	-10.93	-0.0572	0.0200	-10.11	-65.18	-0.82
methylamine	1	-76.40	-75.60	-0.80	0.0261	0.1119	-0.49	-76.09	-0.31
n-propylamine	1	-71.50	-70.56	-0.94	0.0057	0.1097	-0.32	-70.87	-0.63
isopropylamine	1	-69.60	-68.79	-0.81	0.0079	0.1078	-0.17	-68.95	-0.65
tert-butylamine	1	-67.30	-66.05	-1.25	0.0078	0.1061	-0.04	-66.09	-1.21
cyclohexanamine	1	-68.70	-65.87	-2.83	0.0053	0.1063	-0.06	-65.93	-2.77
allylamine	1	-72.00	-70.98	-1.02	-0.0081	0.1123	-0.54	-71.52	-0.48
dimethylamine	1	-68.60	-67.68	-0.92	0.0238	0.1063	-0.06	-67.74	-0.86
diethylamine	1	-63.40	-61.68	-1.72	0.0101	0.1001	0.36	-61.32	-2.08
di-n-propylamine	1	-60.50	-59.29	-1.21	0.0057	0.1000	0.37	-58.92	-1.58
diallylamine	1	-61.60	-60.51	-1.09	-0.0071	0.1021	0.23	-60.28	-1.32
trimethylamine	1	-61.10	-60.96	-0.14	0.0229	0.1021	0.23	-60.73	-0.37
triethylamine	1	-54.60	-53.55	-1.05	0.0065	0.0898	0.92	-52.62	-1.98
aniline	1	-72.40	-70.95	-1.45	0.0005	0.1158	-0.83	-71.78	-0.62
2-methylaniline	1	-70.30	-68.52	-1.78	-0.0004	0.1127	-0.56	-69.08	-1.22
3-methylaniline	1	-69.60	-69.27	-0.33	-0.0008	0.1149	-0.75	-70.02	0.42
4-methylaniline	1	-69.80	-69.08	-0.72	0.0000	0.1143	-0.70	-69.77	-0.03
3-aminoaniline	1	-65.80	-71.65	5.85	-0.0154	0.1150	-0.86	-72.52	6.72
N-methylaniline	1	-62.60	-63.22	0.62	-0.0001	0.1080	-0.18	-63.40	0.80
N-ethylaniline	1	-62.20	-60.42	-1.78	-0.0001	0.1054	0.01	-60.41	-1.79
N,N-dimethylaniline	1	-57.20	-56.69	-0.51	0.0001	0.1009	0.31	-56.37	-0.83
4-methyl-N,N-dimethylaniline	1	-55.90	-55.21	-0.69	-0.0005	0.0998	0.38	-54.82	-1.08
N,N-diethylaniline	1	-54.00	-52.29	-1.71	-0.0009	0.0932	0.75	-51.54	-2.46
1-aminonaphthalene	1	-67.40	-67.83	0.43	-0.0019	0.1165	-0.90	-68.73	1.33
aziridine	1	-70.90	-69.17	-1.73	0.0258	0.1111	-0.43	-69.60	-1.30
azetidine	1	-67.70	-65.43	-2.27	0.0156	0.1038	0.12	-65.31	-2.39
pyrrolidine	1	-66.00	-63.32	-2.68	0.0095	0.1029	0.19	-63.14	-2.86

piperidine	1	-64.20	-61.59	-2.61	0.0106	0.1042	0.09	-61.49	-2.71
azacycloheptane	1	-63.30	-60.02	-3.28	0.0051	0.1041	0.10	-59.91	-3.39
pyrrole	1	-61.40	-61.77	0.37	0.0112	0.1090	-0.26	-62.03	0.63
pyridine	1	-61.10	-60.19	-0.91	0.0140	0.1127	-0.56	-60.75	-0.35
quinoline	1	-56.00	-54.87	-1.13	0.0032	0.1049	0.05	-54.82	-1.18
piperazine	1	-66.00	-63.95	-2.05	-0.0206	0.1046	-0.24	-64.20	-1.80
acetonitrile	1	-75.30	-70.59	-4.71	0.0308	0.1673	-8.90	-79.49	4.19
ammonia	1	-85.20	-85.59	0.39	0.0607	0.1196	-1.19	-86.78	1.58
hydrazine	1	-84.60	-83.34	-1.26	-0.0080	0.1177	-1.02	-84.36	-0.24
methanol	1	-93.00	-82.73	-10.27	0.0141	0.1669	-8.81	-91.54	-1.46
ethanol	1	-88.40	-77.19	-11.21	0.0063	0.1634	-8.01	-85.19	-3.21
dimethyl ether	1	-79.70	-69.61	-10.09	0.0105	0.1567	-6.60	-76.21	-3.49
diethyl ether	1	-71.50	-61.74	-9.76	0.0063	0.1427	-4.10	-65.85	-5.65
acetone	1	-77.10	-67.40	-9.70	0.0042	0.1443	-4.37	-71.77	-5.33
acetophenone	1	-64.50	-56.35	-8.15	0.0006	0.1228	-1.52	-57.87	-6.63
water	1	-110.30	-100.70	-9.60	0.0198	0.1846	-13.57	-114.27	3.97
4-methoxyaniline	1	-71.20	-70.12	-1.08	-0.0203	0.1143	-0.99	-71.11	-0.09
4-nitroaniline	1	-75.90	-84.48	8.58	-0.0183	0.1209	-1.53	-86.00	10.10
morpholine	1	-69.60	-68.27	-1.33	-0.0183	0.1076	-0.36	-68.62	-0.98
acetamide	1	-73.90	-72.37	-1.53	-0.0007	0.1374	-3.32	-75.70	1.80
benzamide	1	-67.20	-64.88	-2.32	-0.0015	0.1336	-2.80	-67.68	0.48
dimethyl sulfide	1	-64.50	-62.46	-2.04	0.0189	0.0806	1.30	-61.16	-3.34
dimethyl sulfoxide	1	-67.70	-64.53	-3.17	-0.0048	0.1326	-2.67	-67.21	-0.49
3-chloroaniline	1	-74.70	-74.01	-0.69	-0.0060	0.1170	-0.94	-74.96	0.26
4-chloroaniline	1	-74.10	-74.28	0.18	-0.0037	0.1185	-1.09	-75.37	1.27
PEARSON			0.99					1.00	

Table S 5-3

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the HF/G3large method for the cavity surface with constant density = 0.002 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.42	2.42	0.0018	0.0351	4.25	3.83	-1.83
ethane	0	1.83	-0.23	2.06	0.0013	0.0315	4.25	4.02	-2.19
n-propane	0	1.96	-0.21	2.17	0.0010	0.0310	4.25	4.04	-2.08
n-butane	0	2.08	-0.17	2.25	0.0008	0.0310	4.25	4.08	-2.00
n-pentane	0	2.33	-0.13	2.46	0.0007	0.0307	4.25	4.13	-1.80
n-hexane	0	2.49	-0.07	2.56	0.0007	0.0310	4.25	4.18	-1.69
n-heptane	0	2.62	-1.18	3.80	0.0006	0.0300	4.25	3.07	-0.45
n-octane	0	2.89	-1.26	4.15	0.0005	0.0307	4.25	2.99	-0.10
2-methylpropane	0	2.32	-0.29	2.61	0.0009	0.0310	4.25	3.96	-1.64
2,2-dimethylpropane	0	2.50	-0.40	2.90	0.0010	0.0311	4.25	3.85	-1.35
2-methylpentane	0	2.52	-1.11	3.63	0.0003	0.0310	4.25	3.14	-0.62
2,4-dimethylpentane	0	2.88	-1.33	4.21	0.0004	0.0317	4.25	2.92	-0.04
2,2,4-trimethylpentane	0	2.85	-1.55	4.40	0.0000	0.0320	4.25	2.70	0.15
cyclopropane	0	0.75	-1.35	2.10	-0.0088	0.0380	4.25	2.90	-2.15
cyclopentane	0	1.20	0.03	1.17	0.0003	0.0301	4.25	4.28	-3.08
cyclohexane	0	1.23	-0.77	2.00	0.0007	0.0286	4.25	3.48	-2.25
methylcyclohexane	0	1.71	-0.96	2.67	0.0005	0.0305	4.25	3.29	-1.58
cis-1,2-dimethylcyclohexane	0	1.58	-1.14	2.72	-0.0002	0.0313	4.25	3.11	-1.53
ethene	0	1.27	-1.91	3.18	-0.0128	0.0445	4.24	2.32	-1.05
propene	0	1.27	-1.76	3.03	-0.0141	0.0416	4.23	2.46	-1.19
1-butene	0	1.38	-1.62	3.00	-0.0146	0.0410	4.22	2.60	-1.22
1-pentene	0	1.66	-1.60	3.26	-0.0146	0.0404	4.22	2.63	-0.97
E-2-pentene	0	1.34	-1.36	2.70	-0.0147	0.0385	4.22	2.86	-1.52
1-hexene	0	1.68	-1.63	3.31	-0.0144	0.0408	4.23	2.59	-0.91
2-methylpropene	0	1.16	-1.71	2.87	-0.0152	0.0389	4.22	2.51	-1.35
s-trans-1,3-butadiene	0	0.61	-3.04	3.65	-0.0108	0.0453	4.24	1.21	-0.60
cyclopentene	0	0.56	-1.12	1.68	-0.0153	0.0426	4.22	3.10	-2.54
ethyne	0	-0.01	-5.97	5.96	-0.0135	0.0879	4.26	-1.70	1.69
propyne	0	-0.31	-4.81	4.50	-0.0165	0.0812	4.23	-0.58	0.27
1-butyne	0	-0.16	-4.57	4.41	-0.0170	0.0811	4.23	-0.34	0.18
1-pentyne	0	0.01	-4.31	4.32	-0.0173	0.0804	4.22	-0.09	0.10
1-hexyne	0	0.29	-4.50	4.79	-0.0170	0.0800	4.22	-0.28	0.57

butenyne	0	0.04	-5.36	5.40	-0.0160	0.0835	4.24	-1.12	1.16
benzene	0	-0.87	-3.45	2.58	-0.0030	0.0462	4.25	0.81	-1.68
ethylbenzene	0	-0.80	-4.42	3.62	-0.0045	0.0452	4.25	-0.17	-0.63
naphthalene	0	-2.39	-6.19	3.80	-0.0052	0.0464	4.25	-1.93	-0.46
anthracene	0	-4.23	-7.94	3.71	-0.0050	0.0473	4.25	-3.69	-0.54
toluene	0	-0.89	-4.33	3.44	-0.0045	0.0453	4.25	-0.07	-0.82
p-xylene	0	-0.81	-4.23	3.42	-0.0057	0.0426	4.25	0.02	-0.83
m-xylene	0	-0.84	-4.28	3.44	-0.0059	0.0447	4.25	-0.03	-0.81
o-xylene	0	-0.90	-4.38	3.48	-0.0058	0.0440	4.25	-0.13	-0.77
fluoromethane	0	-0.22	-3.39	3.17	-0.0236	0.0466	4.07	0.68	-0.90
chloromethane	0	-0.56	-2.37	1.81	-0.0096	0.0522	4.25	1.88	-2.44
bromomethane	0	-0.82	-2.46	1.64	-0.0065	0.0538	4.25	1.79	-2.61
chlorofluoromethane	0	-0.77	-3.66	2.89	-0.0144	0.0655	4.23	0.58	-1.35
dichloromethane	0	-1.36	-2.45	1.09	-0.0037	0.0673	4.26	1.81	-3.17
dibromomethane	0	-2.11	-2.72	0.61	-0.0013	0.0678	4.26	1.55	-3.66
chlorodifluoromethane	0	-0.50	-2.47	1.97	-0.0072	0.0806	4.27	1.81	-2.31
chloroform	0	-1.07	-0.50	-0.57	0.0011	0.0799	4.27	3.78	-4.85
chloroethane	0	-0.63	-2.25	1.62	-0.0109	0.0494	4.25	1.99	-2.62
bromoethane	0	-0.70	-2.38	1.68	-0.0078	0.0513	4.25	1.88	-2.58
bromoform	0	-1.98	-5.64	3.66	0.0025	0.0794	4.27	-1.37	-0.61
tetrafluoromethane	0	3.16	1.36	1.80	0.0004	0.0803	4.27	5.63	-2.47
difluorodichloromethane	0	1.69	2.41	-0.72	-0.0013	0.0609	4.26	6.67	-4.98
fluorotrichloromethane	0	0.82	2.84	-2.02	-0.0024	0.0545	4.26	7.10	-6.28
bromotrifluoromethane	0	1.79	1.40	0.39	-0.0009	0.0787	4.27	5.67	-3.88
bromotrichloromethane	0	-0.93	-3.18	2.25	0.0042	0.0640	4.26	1.08	-2.01
hexafluoroethane	0	3.94	-3.15	7.09	0.0001	0.0808	4.28	1.13	2.81
hexachloroethane	0	-1.40	-3.68	2.28	0.0034	0.0516	4.25	0.57	-1.97
chloropentafluoroethane	0	2.86	-3.02	5.88	-0.0011	0.0759	4.27	1.25	1.61
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-3.19	4.96	-0.0038	0.0594	4.26	1.07	0.70
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-6.91	7.43	-0.0086	0.0826	4.27	-2.64	3.16
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-6.36	6.23	-0.0045	0.0818	4.28	-2.09	1.96
1-chloro-2,2,2-trifluoroethane	0	0.06	-2.48	2.54	-0.0067	0.0688	4.26	1.78	-1.72
1,1,1,2-tetrachloroethane	0	-1.15	-5.95	4.80	-0.0037	0.0662	4.26	-1.69	0.54
1,1,1-trichloroethane	0	-0.25	-4.01	3.76	-0.0016	0.0508	4.25	0.25	-0.50
1,1,2-trichloroethane	0	-1.95	-7.15	5.20	-0.0063	0.0708	4.26	-2.89	0.94

1,1-difluoroethane	0	-0.11	-4.06	3.95	-0.0175	0.0589	4.20	0.14	-0.25
1-bromo-2-chloroethane	0	-1.95	-2.91	0.96	-0.0073	0.0575	4.26	1.35	-3.30
octafluoropropane	0	4.28	-3.80	8.08	0.0002	0.0781	4.27	0.47	3.81
2-chloropropane	0	-0.25	-2.19	1.94	-0.0118	0.0480	4.24	2.05	-2.30
1-chloropropane	0	-0.27	-2.12	1.85	-0.0109	0.0488	4.25	2.12	-2.39
1-bromopropane	0	-0.56	-4.14	3.58	-0.0079	0.0505	4.25	0.11	-0.67
2-bromopropane	0	-0.48	-4.15	3.67	-0.0087	0.0497	4.25	0.10	-0.58
2-chlorobutane	0	0.07	-4.00	4.07	-0.0120	0.0471	4.24	0.24	-0.17
1-bromobutane	0	-0.41	-2.21	1.80	-0.0079	0.0502	4.25	2.04	-2.45
1-chloropentane	0	0.07	-4.38	4.45	-0.0110	0.0486	4.24	-0.14	0.21
2-chloropentane	0	0.07	-4.09	4.16	-0.0120	0.0468	4.24	0.15	-0.08
1-bromopentane	0	-0.08	-4.38	4.30	-0.0080	0.0501	4.25	-0.13	0.05
1-bromo-isobutane	0	-0.03	-4.07	4.04	-0.0079	0.0503	4.25	0.18	-0.21
tetrachloroethene	0	0.05	3.27	-3.22	0.0025	0.0502	4.25	7.53	-7.48
trichloroethene	0	-0.39	0.81	-1.20	-0.0007	0.0731	4.27	5.08	-5.47
chloroethene	0	-0.59	-1.95	1.36	-0.0068	0.0605	4.26	2.31	-2.90
E-1,2-dichloroethene	0	-0.76	-1.05	0.29	-0.0037	0.0677	4.26	3.22	-3.98
Z-1,2-dichloroethene	0	-1.17	-1.84	0.67	-0.0028	0.0684	4.26	2.43	-3.60
3-chloropropene	0	-0.57	-3.13	2.56	-0.0108	0.0534	4.25	1.12	-1.69
3-bromopropene	0	-0.86	-3.65	2.79	-0.0089	0.0553	4.25	0.60	-1.46
fluorobenzene	0	-0.78	-5.21	4.43	-0.0174	0.0531	4.20	-1.01	0.23
chlorobenzene	0	-1.12	-2.44	1.32	-0.0065	0.0526	4.25	1.82	-2.94
bromobenzene	0	-1.46	-4.94	3.48	-0.0041	0.0533	4.26	-0.69	-0.77
1,4-dichlorobenzene	0	-1.01	-5.13	4.12	-0.0050	0.0566	4.26	-0.88	-0.13
1,2-dichlorobenzene	0	-1.36	-1.40	0.04	-0.0057	0.0563	4.26	2.86	-4.22
p-dibromobenzene	0	-2.30	-5.43	3.13	-0.0025	0.0565	4.26	-1.17	-1.13
chlorotoluene	0	-1.92	-7.58	5.66	-0.0105	0.0529	4.25	-3.33	1.41
o-chlorotoluene	0	-1.15	-4.57	3.42	-0.0075	0.0523	4.25	-0.32	-0.83
bromotoluene	0	-2.37	-7.59	5.22	-0.0076	0.0552	4.25	-3.34	0.97
p-bromotoluene	0	-1.39	-4.97	3.58	-0.0046	0.0525	4.25	-0.71	-0.68
2,3-dichlorobiphenyl	0	-2.45	-7.71	5.26	-0.0063	0.0551	4.26	-3.46	1.01
2,2'-dichlorobiphenyl	0	-2.73	-8.13	5.40	-0.0075	0.0519	4.25	-3.88	1.15
2,2',3'-trichlorobiphenyl	0	-1.99	-8.13	6.14	-0.0076	0.0555	4.25	-3.88	1.89
1,2-dimethoxyethane	0	-4.84	-5.56	0.72	-0.0346	0.0383	3.44	-2.12	-2.72
anisole	0	-2.45	-6.79	4.34	-0.0303	0.0483	3.77	-3.02	0.57

dimethyl ether	0	-1.92	-3.71	1.79	-0.0357	0.0386	3.34	-0.37	-1.55
diethyl ether	0	-1.76	-3.73	1.97	-0.0372	0.0362	3.18	-0.54	-1.22
isopropyl ether	0	-0.53	-4.72	4.19	-0.0377	0.0362	3.12	-1.61	1.08
methyl propyl ether	0	-1.66	-3.39	1.73	-0.0358	0.0379	3.33	-0.06	-1.60
methyl isopropyl ether	0	-2.01	-4.46	2.45	-0.0365	0.0372	3.26	-1.20	-0.81
t-butyl methyl ether	0	-2.21	-4.54	2.33	-0.0367	0.0365	3.23	-1.31	-0.90
ethyl phenyl ether	0	-2.22	-6.68	4.46	-0.0304	0.0481	3.76	-2.92	0.70
tetrahydrofuran	0	-3.47	-3.88	0.41	-0.0379	0.0376	3.09	-0.78	-2.69
tetrahydropyran	0	-3.12	-4.62	1.50	-0.0374	0.0357	3.15	-1.47	-1.65
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-8.26	8.14	-0.0217	0.0689	4.13	-4.13	4.01
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-10.25	10.36	-0.0134	0.0828	4.26	-5.99	6.10
acetaldehyde	0	-3.50	-8.35	4.85	-0.0370	0.0634	3.21	-5.14	1.64
propanal	0	-3.44	-7.75	4.31	-0.0373	0.0602	3.18	-4.57	1.13
butanal	0	-3.18	-7.89	4.71	-0.0371	0.0615	3.19	-4.70	1.52
pentanal	0	-3.03	-8.80	5.77	-0.0376	0.0588	3.13	-5.67	2.64
octanal	0	-2.29	-8.62	6.33	-0.0373	0.0577	3.17	-5.45	3.16
benzaldehyde	0	-4.02	-10.56	6.54	-0.0379	0.0578	3.11	-7.46	3.44
p-hydroxybenzaldehyde	0	-10.48	-17.89	7.41	-0.0389	0.1388	3.18	-14.71	4.23
m-hydroxybenzaldehyde	0	-9.51	-17.32	7.81	-0.0377	0.1396	3.33	-14.00	4.49
acetone	0	-3.85	-8.38	4.53	-0.0391	0.0573	2.96	-5.43	1.58
2-butanone	0	-3.64	-7.78	4.14	-0.0396	0.0562	2.89	-4.89	1.25
2-pentanone	0	-3.53	-8.84	5.31	-0.0394	0.0551	2.91	-5.93	2.40
3-pentanone	0	-3.41	-8.30	4.89	-0.0379	0.0551	3.10	-5.20	1.79
2-hexanone	0	-3.29	-8.96	5.67	-0.0396	0.0548	2.89	-6.07	2.78
2-heptanone	0	-3.04	-9.06	6.02	-0.0394	0.0523	2.91	-6.16	3.12
4-heptanone	0	-2.93	-8.52	5.59	-0.0382	0.0549	3.06	-5.46	2.53
2-octanone	0	-2.88	-9.02	6.14	-0.0393	0.0498	2.93	-6.09	3.21
5-nonanone	0	-2.67	-8.57	5.90	-0.0381	0.0541	3.08	-5.49	2.82
3,3-dimethylbutanone	0	-2.89	-8.57	5.68	-0.0397	0.0516	2.88	-5.70	2.81
cyclopentanone	0	-4.68	-9.37	4.69	-0.0389	0.0566	2.97	-6.40	1.72
acetophenone	0	-4.58	-10.48	5.90	-0.0393	0.0538	2.92	-7.56	2.98
methyl formate	0	-2.78	-8.30	5.52	-0.0340	0.0687	3.51	-4.79	2.01
ethyl formate	0	-2.65	-8.11	5.46	-0.0345	0.0670	3.46	-4.65	2.00
methyl acetate	0	-3.32	-7.75	4.43	-0.0364	0.0638	3.27	-4.48	1.16
ethyl acetate	0	-3.10	-8.93	5.83	-0.0368	0.0622	3.23	-5.70	2.60

propyl acetate	0	-2.86	-8.98	6.12	-0.0370	0.0633	3.21	-5.77	2.91
butyl acetate	0	-2.55	-9.08	6.53	-0.0369	0.0623	3.22	-5.86	3.31
methyl propanoate	0	-2.93	-7.28	4.35	-0.0360	0.0625	3.31	-3.96	1.03
methyl butanoate	0	-2.83	-8.70	5.87	-0.0363	0.0619	3.29	-5.41	2.58
methyl pentanoate	0	-2.57	-8.79	6.22	-0.0360	0.0609	3.31	-5.48	2.91
methyl hexanoate	0	-2.49	-8.90	6.41	-0.0364	0.0602	3.27	-5.63	3.14
methyl benzoate	0	-3.91	-9.70	5.79	-0.0370	0.0599	3.20	-6.50	2.59
hydrogen	0	2.33	-0.49	2.82	0.0020	0.0401	4.25	3.77	-1.44
water	0	-6.31	-11.16	4.85	-0.0356	0.1265	3.49	-7.67	1.36
water dimer	0	-11.27	-17.49	6.22	-0.0400	0.1328	3.00	-14.49	3.22
hydrogen peroxide	0	-8.58	-13.02	4.44	-0.0288	0.1431	4.08	-8.94	0.36
methyl peroxide	0	-5.28	-9.16	3.88	-0.0297	0.1404	4.02	-5.14	-0.14
ethyl peroxide	0	-5.32	-9.05	3.73	-0.0302	0.1372	3.97	-5.08	-0.24
1,4-dioxane	0	-5.05	-6.50	1.45	-0.0351	0.0419	3.39	-3.11	-1.94
methanol	0	-5.11	-7.60	2.49	-0.0360	0.1209	3.42	-4.18	-0.93
ethanol	0	-5.01	-7.23	2.22	-0.0362	0.1190	3.40	-3.83	-1.18
1-propanol	0	-4.83	-7.15	2.32	-0.0362	0.1175	3.39	-3.76	-1.07
isopropanol	0	-4.76	-7.18	2.42	-0.0370	0.1150	3.29	-3.88	-0.88
1-butanol	0	-4.72	-7.11	2.39	-0.0362	0.1172	3.39	-3.72	-1.00
t-butanol	0	-4.51	-6.95	2.44	-0.0369	0.1124	3.31	-3.65	-0.86
1-pentanol	0	-4.47	-8.42	3.95	-0.0367	0.1151	3.33	-5.09	0.62
1-hexanol	0	-4.36	-8.59	4.23	-0.0370	0.1183	3.31	-5.28	0.92
1-heptanol	0	-4.24	-8.18	3.94	-0.0369	0.1121	3.30	-4.88	0.64
1-octanol	0	-4.09	-8.35	4.26	-0.0365	0.1124	3.35	-5.01	0.92
allyl alcohol	0	-5.08	-7.95	2.87	-0.0357	0.1200	3.45	-4.50	-0.58
cyclopentanol	0	-5.49	-7.71	2.22	-0.0371	0.1094	3.28	-4.43	-1.06
2-methoxyethanol	0	-6.77	-10.04	3.27	-0.0351	0.1228	3.52	-6.51	-0.26
2,2,2-trifluoroethanol	0	-4.31	-12.81	8.50	-0.0275	0.1349	4.10	-8.71	4.40
1,1,1-trifluoropropan-2-ol	0	-4.16	-9.96	5.80	-0.0305	0.1303	3.91	-6.04	1.88
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-12.03	8.26	-0.0232	0.1459	4.33	-7.70	3.93
phenol	0	-6.62	-9.85	3.23	-0.0288	0.1333	4.03	-5.82	-0.80
p-bromophenol	0	-7.13	-11.98	4.85	-0.0265	0.1345	4.15	-7.83	0.70
o-cresol	0	-5.87	-10.56	4.69	-0.0290	0.1322	4.01	-6.55	0.68
m-cresol	0	-5.49	-11.04	5.55	-0.0291	0.1368	4.03	-7.01	1.52
p-cresol	0	-6.14	-10.96	4.82	-0.0294	0.1359	4.01	-6.95	0.81

1,2-ethanediol	0	-9.30	-12.16	2.86	-0.0378	0.1277	3.26	-8.90	-0.40
acetic acid	0	-6.70	-11.93	5.23	-0.0354	0.1490	3.63	-8.30	1.60
propanoic acid	0	-6.47	-11.44	4.97	-0.0350	0.1474	3.66	-7.78	1.31
butanoic acid	0	-6.36	-11.35	4.99	-0.0351	0.1477	3.65	-7.69	1.33
pentanoic acid	0	-6.16	-12.88	6.72	-0.0350	0.1490	3.67	-9.20	3.04
hexanoic acid	0	-6.21	-12.96	6.75	-0.0353	0.1463	3.63	-9.33	3.12
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-21.16	9.20	-0.0316	0.1513	3.97	-17.18	5.22
ammonia	0	-4.29	-6.76	2.47	-0.0407	0.0736	2.75	-4.01	-0.28
methylamine	0	-4.56	-5.32	0.76	-0.0409	0.0700	2.71	-2.61	-1.95
ethylamine	0	-4.50	-5.36	0.86	-0.0412	0.0686	2.66	-2.69	-1.81
butylamine	0	-4.29	-6.20	1.91	-0.0412	0.0680	2.67	-3.53	-0.76
propylamine	0	-4.39	-5.32	0.93	-0.0411	0.0687	2.69	-2.64	-1.75
pentylamine	0	-4.10	-6.35	2.25	-0.0412	0.0676	2.66	-3.69	-0.41
dimethylamine	0	-4.29	-3.85	-0.44	-0.0398	0.0690	2.87	-0.97	-3.32
diethylamine	0	-4.07	-3.63	-0.44	-0.0398	0.0660	2.86	-0.77	-3.30
dipropylamine	0	-3.66	-4.70	1.04	-0.0396	0.0657	2.89	-1.81	-1.85
trimethylamine	0	-3.23	-2.34	-0.89	-0.0384	0.0349	3.04	0.70	-3.93
azetidine	0	-5.56	-4.06	-1.50	-0.0413	0.0668	2.65	-1.41	-4.15
pyrrolidine	0	-5.48	-5.18	-0.30	-0.0414	0.0666	2.63	-2.55	-2.93
piperidine	0	-5.11	-4.10	-1.01	-0.0396	0.0673	2.90	-1.20	-3.91
2-methoxyethanamine	0	-6.55	-8.47	1.92	-0.0397	0.0707	2.88	-5.59	-0.96
1,2-ethanediamine	0	-9.72	-10.44	0.72	-0.0399	0.0709	2.85	-7.59	-2.13
nitromethane	0	-3.95	-10.42	6.47	-0.0269	0.0651	3.96	-6.46	2.51
nitroethane	0	-3.71	-9.64	5.93	-0.0278	0.0612	3.92	-5.73	2.02
1-nitropropane	0	-3.34	-9.41	6.07	-0.0277	0.0603	3.92	-5.49	2.15
2-nitropropane	0	-3.14	-8.60	5.46	-0.0282	0.0587	3.89	-4.71	1.57
1-nitrobutane	0	-3.08	-10.97	7.89	-0.0278	0.0608	3.92	-7.05	3.97
nitrobenzene	0	-4.12	-10.10	5.98	-0.0266	0.0624	3.97	-6.13	2.01
2-methyl-1-nitrobenzene	0	-3.59	-9.61	6.02	-0.0280	0.0598	3.90	-5.71	2.12
pyridine	0	-4.70	-6.99	2.29	-0.0399	0.0550	2.85	-4.14	-0.56
2-methylpyridine	0	-4.63	-6.66	2.03	-0.0404	0.0529	2.78	-3.89	-0.74
3-methylpyridine	0	-4.77	-6.98	2.21	-0.0404	0.0522	2.77	-4.21	-0.56
4-methylpyridine	0	-4.94	-6.10	1.16	-0.0409	0.0488	2.70	-3.41	-1.53
4-ethylpyridine	0	-4.74	-7.23	2.49	-0.0409	0.0492	2.70	-4.53	-0.21
2,4-dimethylpyridine	0	-4.86	-6.88	2.02	-0.0414	0.0473	2.62	-4.26	-0.60

2,5-dimethylpyridine	0	-4.72	-6.64	1.92	-0.0407	0.0512	2.73	-3.91	-0.81
2,6-dimethylpyridine	0	-4.60	-6.37	1.77	-0.0408	0.0531	2.72	-3.65	-0.95
3,4-dimethylpyridine	0	-5.22	-7.29	2.07	-0.0414	0.0486	2.63	-4.66	-0.56
3,5-dimethylpyridine	0	-4.84	-6.97	2.13	-0.0409	0.0511	2.70	-4.28	-0.56
aniline	0	-5.49	-9.82	4.33	-0.0309	0.0865	3.76	-6.06	0.57
N-methylaniline	0	-4.68	-7.97	3.29	-0.0278	0.0848	3.94	-4.03	-0.65
2-methylaniline	0	-5.56	-9.24	3.68	-0.0318	0.0831	3.70	-5.54	-0.02
3-methylaniline	0	-5.67	-9.72	4.05	-0.0315	0.0859	3.72	-6.00	0.33
4-methylaniline	0	-5.55	-9.60	4.05	-0.0319	0.0830	3.69	-5.91	0.36
N-ethylaniline	0	-4.62	-7.87	3.25	-0.0252	0.0863	4.05	-3.82	-0.80
3-aminoaniline	0	-9.92	-15.22	5.30	-0.0312	0.0859	3.74	-11.48	1.56
N,N-dimethylaniline	0	-3.58	-6.18	2.60	-0.0229	0.0443	4.09	-2.08	-1.50
piperazine	0	-7.40	-7.34	-0.06	-0.0394	0.0684	2.93	-4.42	-2.98
N-methylpiperazine	0	-7.77	-6.11	-1.66	-0.0391	0.0689	2.96	-3.14	-4.63
N,N'-dimethylpiperazine	0	-7.58	-4.84	-2.74	-0.0377	0.0346	3.12	-1.72	-5.86
1-methylthymine	0	-10.40	-20.34	9.94	-0.0393	0.1196	3.04	-17.30	6.90
9-methyladenine	0	-13.60	-17.89	4.29	-0.0446	0.1058	2.14	-15.75	2.15
acetamide	0	-9.71	-14.13	4.42	-0.0426	0.1046	2.50	-11.63	1.92
E-N-methylacetamide	0	-10.00	-13.36	3.36	-0.0440	0.0953	2.22	-11.13	1.13
Z-N-methylacetamide	0	-10.00	-12.64	2.64	-0.0440	0.1031	2.24	-10.40	0.40
benzamide	0	-10.90	-15.84	4.94	-0.0423	0.1049	2.56	-13.29	2.39
2,6-dichlorothiobenzamide	0	-10.81	-18.21	7.40	-0.0294	0.1218	3.94	-14.27	3.46
urea	0	-13.80	-17.87	4.07	-0.0419	0.1026	2.60	-15.27	1.47
1,1-dimethyl-3-phenylurea	0	-9.63	-14.61	4.98	-0.0400	0.0998	2.88	-11.73	2.10
hydrazine	0	-6.26	-9.50	3.24	-0.0388	0.0746	3.01	-6.49	0.23
methylhydrazine	0	-5.31	-8.29	2.98	-0.0388	0.0736	3.01	-5.29	-0.02
1,1-dimethylhydrazine	0	-4.48	-7.56	3.08	-0.0391	0.0740	2.96	-4.60	0.12
2-methylpyrazine	0	-5.57	-7.43	1.86	-0.0351	0.0551	3.40	-4.03	-1.54
2-ethylpyrazine	0	-5.51	-7.05	1.54	-0.0350	0.0545	3.41	-3.64	-1.87
morpholine	0	-7.17	-6.47	-0.70	-0.0378	0.0713	3.12	-3.35	-3.82
N-methylmorpholine	0	-6.34	-6.40	0.06	-0.0366	0.0385	3.25	-3.15	-3.19
acetonitrile	0	-3.89	-9.35	5.46	-0.0345	0.0593	3.45	-5.89	2.00
butanonitrile	0	-3.64	-9.20	5.56	-0.0345	0.0549	3.46	-5.74	2.10
propionitrile	0	-3.85	-8.73	4.88	-0.0347	0.0552	3.44	-5.29	1.44
benzonitrile	0	-4.10	-10.25	6.15	-0.0337	0.0587	3.53	-6.73	2.63

2,6-dichlorobenzonitrile	0	-5.22	-10.71	5.49	-0.0323	0.0634	3.64	-7.07	1.85
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-14.98	5.98	-0.0322	0.1238	3.77	-11.21	2.21
trimethylphosphate	0	-8.70	-14.68	5.98	-0.0406	0.0761	2.76	-11.92	3.22
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-14.62	8.01	-0.0363	0.0861	3.30	-11.31	4.70
phosphine	0	0.60	-1.18	1.78	-0.0125	0.0472	4.24	3.06	-2.46
hydrogen sulfide	0	-0.70	-3.23	2.53	-0.0129	0.0669	4.25	1.01	-1.71
dimethyl sulfide	0	-1.54	-3.30	1.76	-0.0213	0.0446	4.13	0.83	-2.37
diethyl sulfide	0	-1.43	-2.88	1.45	-0.0225	0.0387	4.10	1.22	-2.65
dipropyl sulfide	0	-1.27	-4.51	3.24	-0.0226	0.0383	4.10	-0.41	-0.86
bis(2-chloroethyl)sulfide	0	-3.92	-9.50	5.58	-0.0162	0.0540	4.21	-5.29	1.37
dimethyl disulfide	0	-1.83	-3.41	1.58	-0.0158	0.0480	4.22	0.81	-2.64
diethyl disulfide	0	-1.63	-4.87	3.24	-0.0163	0.0449	4.21	-0.66	-0.97
methanethiol	0	-1.24	-3.27	2.03	-0.0177	0.0598	4.20	0.93	-2.17
ethanethiol	0	-1.30	-3.14	1.84	-0.0182	0.0583	4.19	1.05	-2.35
1-propanethiol	0	-1.05	-4.30	3.25	-0.0182	0.0580	4.19	-0.11	-0.94
thiophene	0	-1.42	-3.78	2.36	-0.0070	0.0584	4.26	0.48	-1.90
thiophenol	0	-2.55	-6.77	4.22	-0.0124	0.0656	4.25	-2.52	-0.03
thioanisole	0	-2.73	-6.86	4.13	-0.0164	0.0486	4.21	-2.65	-0.08
tetramethylsilane	0	3.04	-2.08	5.12	-0.0008	0.0391	4.25	2.17	0.87
acetylene	-1	-76.50	-72.88	-3.62	-0.0649	0.0482	-5.14	-78.02	1.52
acetonitrile	-1	-66.60	-64.96	-1.64	-0.0600	0.0187	-2.67	-67.64	1.04
cyanamide	-1	-72.20	-69.83	-2.37	-0.0601	0.0515	-2.71	-72.54	0.34
aniline	-1	-62.90	-61.24	-1.66	-0.0668	0.0309	-6.27	-67.51	4.61
diphenylamine	-1	-54.60	-53.93	-0.67	-0.0603	0.0336	-2.82	-56.75	2.15
hydrogen cyanide	-1	-70.20	-71.24	1.04	-0.0597	-0.0323	-2.53	-73.77	3.57
formic acid	-1	-76.20	-72.23	-3.97	-0.0622	0.0250	-3.71	-75.95	-0.25
acetic acid	-1	-77.60	-71.99	-5.61	-0.0638	0.0253	-4.55	-76.54	-1.06
propanoic acid	-1	-76.20	-69.87	-6.33	-0.0639	0.0266	-4.62	-74.49	-1.71
hexanoic acid	-1	-74.60	-69.31	-5.29	-0.0640	0.0280	-4.67	-73.98	-0.62
acrylic acid	-1	-74.00	-70.67	-3.33	-0.0636	0.0392	-4.41	-75.08	1.08
pyruvic acid	-1	-68.50	-70.58	2.08	-0.0597	0.0512	-2.55	-73.14	4.64
benzoic acid	-1	-71.20	-68.03	-3.17	-0.0627	0.0420	-3.94	-71.98	0.78
methanol	-1	-95.00	-74.81	-20.19	-0.0767	-0.0074	-13.79	-88.61	-6.39
ethanol	-1	-90.70	-72.15	-18.55	-0.0775	0.0171	-14.49	-86.64	-4.06
1-propanol	-1	-88.30	-71.45	-16.85	-0.0776	0.0227	-14.60	-86.04	-2.26

isopropanol	-1	-86.30	-69.80	-16.50	-0.0771	0.0169	-14.19	-84.00	-2.30
2-butanol	-1	-84.20	-66.18	-18.02	-0.0768	0.0163	-13.92	-80.10	-4.10
t-butanol	-1	-82.30	-67.78	-14.52	-0.0764	0.0173	-13.55	-81.33	-0.97
allyl alcohol	-1	-86.60	-71.37	-15.23	-0.0773	0.0293	-14.33	-85.70	-0.90
benzyl alcohol	-1	-85.10	-66.89	-18.21	-0.0759	0.0373	-13.08	-79.96	-5.14
2-methoxyethanol	-1	-89.40	-73.37	-16.03	-0.0771	0.0309	-14.20	-87.57	-1.83
phenol	-1	-71.90	-63.56	-8.34	-0.0675	0.0320	-6.73	-70.29	-1.61
2-methylphenol	-1	-70.20	-61.70	-8.50	-0.0681	0.0297	-7.08	-68.78	-1.42
3-methylphenol	-1	-71.10	-63.59	-7.51	-0.0678	0.0312	-6.93	-70.51	-0.59
4-methylphenol	-1	-72.00	-63.60	-8.40	-0.0684	0.0301	-7.32	-70.92	-1.08
1,2-ethanediol	-1	-85.30	-77.65	-7.65	-0.0772	0.1068	-14.20	-91.85	6.55
3-hydroxyphenol	-1	-73.80	-67.35	-6.45	-0.0665	0.1197	-5.98	-73.33	-0.47
4-hydroxyphenol	-1	-77.60	-69.69	-7.91	-0.0688	0.1152	-7.45	-77.14	-0.46
methyl hydroperoxide	-1	-93.20	-77.90	-15.30	-0.0761	0.0195	-13.28	-91.18	-2.02
ethyl hydroperoxide	-1	-89.20	-77.16	-12.04	-0.0764	0.0269	-13.50	-90.66	1.46
acetaldehyde	-1	-76.50	-68.28	-8.22	-0.0686	0.0164	-7.41	-75.68	-0.82
acetone	-1	-76.20	-67.46	-8.74	-0.0693	0.0220	-7.88	-75.35	-0.85
3-pentanone	-1	-73.70	-61.89	-11.81	-0.0683	0.0201	-7.22	-69.11	-4.59
water	-1	-104.70	-88.28	-16.42	-0.0826	0.0288	-19.78	-108.06	3.36
hydrogen peroxide	-1	-97.30	-84.59	-12.71	-0.0759	0.0837	-13.03	-97.62	0.32
hydroperoxyl radical	-1	-83.30	-78.15	-5.15	-0.0652	-0.0459	-5.33	-83.48	0.18
2-nitrophenol	-1	-60.10	-61.50	1.40	-0.0604	0.0465	-2.85	-64.36	4.26
3-nitrophenol	-1	-61.90	-58.28	-3.62	-0.0638	0.0542	-4.54	-62.82	0.92
4-nitrophenol	-1	-57.80	-56.11	-1.69	-0.0583	0.0489	-1.93	-58.04	0.24
nitromethane	-1	-76.50	-69.72	-6.78	-0.0609	0.0356	-3.10	-72.82	-3.68
4-nitroaniline	-1	-57.40	-55.53	-1.87	-0.0567	0.0475	-1.28	-56.81	-0.59
acetamide	-1	-80.20	-69.41	-10.79	-0.0650	0.0305	-5.22	-74.63	-5.57
methanethiol	-1	-73.80	-67.55	-6.25	-0.0516	0.0171	0.41	-67.14	-6.66
ethanethiol	-1	-71.80	-65.77	-6.03	-0.0519	0.0229	0.33	-65.44	-6.36
1-propanethiol	-1	-70.50	-65.57	-4.93	-0.0519	0.0259	0.32	-65.26	-5.24
thiophenol	-1	-63.40	-60.92	-2.48	-0.0473	0.0373	1.52	-59.41	-3.99
hydrogen sulfide	-1	-72.10	-68.71	-3.39	-0.0488	0.0162	1.16	-67.55	-4.55
dimethyl sulfoxide	-1	-67.70	-65.87	-1.83	-0.0649	0.0335	-5.13	-70.99	3.29
hydrofluoric acid	-1	-104.40	-93.79	-10.61	-0.0856	-0.0856	-23.44	-117.23	12.83
hydrochloric acid	-1	-74.50	-72.93	-1.57	-0.0476	-0.0476	1.44	-71.49	-3.01

hydrobromic acid	-1	-68.30	-67.68	-0.62	-0.0395	-0.0395	2.90	-64.78	-3.52
chloroform	-1	-54.10	-52.69	-1.41	-0.0448	0.0062	2.04	-50.65	-3.45
trifluoroacetic acid	-1	-59.30	-63.16	3.86	-0.0555	0.0650	-0.83	-63.99	4.69
chloroacetic acid	-1	-69.70	-66.76	-2.94	-0.0595	0.0415	-2.44	-69.20	-0.50
dichloroacetic acid	-1	-62.30	-62.41	0.11	-0.0564	0.0530	-1.17	-63.57	1.27
2,2,2-trifluoroethanol	-1	-77.50	-66.76	-10.74	-0.0723	0.0409	-10.09	-76.85	-0.65
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-61.29	-4.21	-0.0671	0.0462	-6.45	-67.74	2.24
2-chlorophenol	-1	-66.10	-60.51	-5.59	-0.0650	0.0394	-5.23	-65.74	-0.36
4-chlorophenol	-1	-66.00	-58.92	-7.08	-0.0656	0.0397	-5.53	-64.44	-1.56
methylamine	1	-76.40	-83.29	6.89	0.0301	0.1510	4.53	-78.76	2.36
n-propylamine	1	-71.50	-78.36	6.86	0.0043	0.1482	4.52	-73.84	2.34
isopropylamine	1	-69.60	-76.63	7.03	0.0043	0.1463	4.50	-72.13	2.53
tert-butylamine	1	-67.30	-74.00	6.70	0.0054	0.1453	4.50	-69.51	2.21
cyclohexanamine	1	-68.70	-73.69	4.99	0.0039	0.1458	4.50	-69.19	0.49
allylamine	1	-72.00	-79.33	7.33	-0.0154	0.1524	4.51	-74.82	2.82
dimethylamine	1	-68.60	-74.63	6.03	0.0282	0.1454	4.50	-70.13	1.53
diethylamine	1	-63.40	-68.70	5.30	0.0048	0.1391	4.46	-64.25	0.85
di-n-propylamine	1	-60.50	-66.66	6.16	0.0083	0.1394	4.46	-62.20	1.70
diallylamine	1	-61.60	-68.77	7.17	-0.0134	0.1419	4.45	-64.31	2.71
trimethylamine	1	-61.10	-67.11	6.01	0.0271	0.1417	4.47	-62.64	1.54
triethylamine	1	-54.60	-59.79	5.19	0.0053	0.1288	4.40	-55.38	0.78
aniline	1	-72.40	-80.30	7.90	0.0036	0.1572	4.58	-75.72	3.32
2-methylaniline	1	-70.30	-77.91	7.61	-0.0017	0.1548	4.56	-73.35	3.05
3-methylaniline	1	-69.60	-78.49	8.89	0.0022	0.1585	4.59	-73.90	4.30
4-methylaniline	1	-69.80	-78.35	8.55	0.0027	0.1575	4.59	-73.77	3.97
3-aminoaniline	1	-65.80	-82.43	16.63	-0.0191	0.1581	4.51	-77.92	12.12
N-methylaniline	1	-62.60	-71.65	9.05	0.0031	0.1493	4.52	-67.13	4.53
N-ethylaniline	1	-62.20	-68.72	6.52	0.0039	0.1462	4.50	-64.22	2.02
N,N-dimethylaniline	1	-57.20	-63.92	6.72	0.0033	0.1420	4.47	-59.45	2.25
4-methyl-N,N-dimethylaniline	1	-55.90	-62.35	6.45	0.0026	0.1393	4.46	-57.90	2.00
N,N-diethylaniline	1	-54.00	-59.38	5.38	0.0024	0.1332	4.42	-54.95	0.95
1-aminonaphthalene	1	-67.40	-77.63	10.23	0.0001	0.1582	4.59	-73.04	5.64
aziridine	1	-70.90	-76.24	5.34	0.0294	0.1517	4.54	-71.70	0.80
azetidine	1	-67.70	-72.08	4.38	0.0179	0.1418	4.47	-67.61	-0.09
pyrrolidine	1	-66.00	-70.00	4.00	0.0092	0.1409	4.47	-65.53	-0.47

piperidine	1	-64.20	-68.36	4.16	0.0054	0.1438	4.49	-63.87	-0.33
azacycloheptane	1	-63.30	-66.89	3.59	-0.0025	0.1432	4.48	-62.40	-0.90
pyrrole	1	-61.40	-68.48	7.08	0.0129	0.1513	4.54	-63.95	2.55
pyridine	1	-61.10	-66.92	5.82	0.0179	0.1568	4.58	-62.34	1.24
quinoline	1	-56.00	-61.85	5.85	0.0055	0.1469	4.51	-57.34	1.34
piperazine	1	-66.00	-71.84	5.84	-0.0287	0.1443	4.10	-67.75	1.75
acetonitrile	1	-75.30	-78.95	3.65	0.0360	0.2303	5.73	-73.22	-2.08
ammonia	1	-85.20	-94.18	8.98	0.0692	0.1602	4.61	-89.57	4.37
hydrazine	1	-84.60	-93.13	8.53	-0.0133	0.1588	4.58	-88.55	3.95
methanol	1	-93.00	-92.63	-0.37	0.0135	0.2284	5.68	-86.95	-6.05
ethanol	1	-88.40	-86.91	-1.49	-0.0056	0.2243	5.58	-81.33	-7.07
dimethyl ether	1	-79.70	-77.38	-2.32	0.0098	0.2173	5.43	-71.96	-7.74
diethyl ether	1	-71.50	-69.37	-2.13	0.0053	0.2023	5.14	-64.23	-7.27
acetone	1	-77.10	-76.10	-1.00	0.0033	0.2027	5.15	-70.96	-6.14
acetophenone	1	-64.50	-64.60	0.10	-0.0007	0.1719	4.72	-59.87	-4.63
water	1	-110.30	-113.13	2.83	0.0197	0.2486	6.24	-106.89	-3.41
4-methoxyaniline	1	-71.20	-80.09	8.89	-0.0249	0.1532	4.33	-75.76	4.56
4-nitroaniline	1	-75.90	-96.08	20.18	-0.0209	0.1615	4.51	-91.57	15.67
morpholine	1	-69.60	-76.61	7.01	-0.0239	0.1479	4.32	-72.29	2.69
acetamide	1	-73.90	-82.06	8.16	-0.0025	0.1936	5.00	-77.06	3.16
benzamide	1	-67.20	-74.91	7.71	-0.0052	0.1880	4.92	-69.99	2.79
dimethyl sulfide	1	-64.50	-68.89	4.39	0.0226	0.1125	4.34	-64.55	0.05
dimethyl sulfoxide	1	-67.70	-72.94	5.24	-0.0077	0.1875	4.91	-68.03	0.33
3-chloroaniline	1	-74.70	-83.87	9.17	-0.0048	0.1593	4.60	-79.27	4.57
4-chloroaniline	1	-74.10	-84.26	10.16	-0.0027	0.1596	4.60	-79.66	5.56
PEARSON			0.99					1.00	

Table S 6-1

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/G3large method for the cavity surface with constant density = 0.0005 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.15	2.15	-0.0009	0.0112	1.46	1.32	0.68
ethane	0	1.83	-0.14	1.97	-0.0013	0.0095	1.47	1.33	0.50
n-propane	0	1.96	-0.18	2.14	-0.0014	0.0094	1.47	1.30	0.66
n-butane	0	2.08	-0.21	2.29	-0.0015	0.0095	1.47	1.26	0.82
n-pentane	0	2.33	-0.24	2.57	-0.0015	0.0094	1.47	1.23	1.10
n-hexane	0	2.49	-0.27	2.76	-0.0016	0.0093	1.47	1.20	1.29
n-heptane	0	2.62	-0.30	2.92	-0.0016	0.0090	1.47	1.18	1.44
n-octane	0	2.89	-0.33	3.22	-0.0015	0.0089	1.47	1.15	1.74
2-methylpropane	0	2.32	-0.24	2.56	-0.0014	0.0094	1.47	1.23	1.09
2,2-dimethylpropane	0	2.50	-0.31	2.81	-0.0013	0.0094	1.47	1.16	1.34
2-methylpentane	0	2.52	-0.27	2.79	-0.0016	0.0093	1.47	1.20	1.32
2,4-dimethylpentane	0	2.88	-0.34	3.22	-0.0016	0.0096	1.47	1.13	1.75
2,2,4-trimethylpentane	0	2.85	-0.40	3.25	-0.0018	0.0104	1.47	1.07	1.78
cyclopropane	0	0.75	-0.61	1.36	-0.0077	0.0124	1.35	0.73	0.02
cyclopentane	0	1.20	-0.20	1.40	-0.0019	0.0091	1.47	1.27	-0.07
cyclohexane	0	1.23	-0.17	1.40	-0.0016	0.0083	1.48	1.31	-0.08
methylcyclohexane	0	1.71	-0.23	1.94	-0.0016	0.0091	1.47	1.24	0.47
cis-1,2-dimethylcyclohexane	0	1.58	-0.27	1.85	-0.0016	0.0096	1.47	1.20	0.38
ethene	0	1.27	-0.77	2.04	-0.0091	0.0151	1.25	0.48	0.79
propene	0	1.27	-0.77	2.04	-0.0099	0.0136	1.22	0.46	0.81
1-butene	0	1.38	-0.74	2.12	-0.0101	0.0130	1.21	0.47	0.91
1-pentene	0	1.66	-0.78	2.44	-0.0102	0.0129	1.21	0.43	1.23
E-2-pentene	0	1.34	-0.64	1.98	-0.0099	0.0120	1.24	0.59	0.75
1-hexene	0	1.68	-0.84	2.52	-0.0101	0.0131	1.21	0.37	1.31
2-methylpropene	0	1.16	-0.79	1.95	-0.0104	0.0120	1.20	0.41	0.75
s-trans-1,3-butadiene	0	0.61	-1.28	1.89	-0.0078	0.0154	1.31	0.03	0.58
cyclopentene	0	0.56	-0.61	1.17	-0.0101	0.0139	1.20	0.60	-0.04
ethyne	0	-0.01	-2.46	2.45	-0.0097	0.0353	0.56	-1.90	1.89
propyne	0	-0.31	-2.15	1.84	-0.0117	0.0309	0.63	-1.52	1.21
1-butyne	0	-0.16	-2.04	1.88	-0.0119	0.0309	0.62	-1.42	1.26
1-pentyne	0	0.01	-1.93	1.94	-0.0120	0.0306	0.63	-1.30	1.31
1-hexyne	0	0.29	-2.12	2.41	-0.0121	0.0302	0.64	-1.48	1.77

butenyne	0	0.04	-2.22	2.26	-0.0107	0.0331	0.61	-1.61	1.65
benzene	0	-0.87	-1.63	0.76	-0.0055	0.0157	1.38	-0.25	-0.62
ethylbenzene	0	-0.80	-1.60	0.80	-0.0065	0.0150	1.36	-0.23	-0.57
naphthalene	0	-2.39	-2.29	-0.10	-0.0056	0.0160	1.37	-0.92	-1.47
anthracene	0	-4.23	-2.92	-1.31	-0.0056	0.0159	1.37	-1.55	-2.68
toluene	0	-0.89	-1.59	0.70	-0.0065	0.0150	1.36	-0.23	-0.66
p-xylene	0	-0.81	-1.51	0.70	-0.0072	0.0138	1.35	-0.16	-0.65
m-xylene	0	-0.84	-1.53	0.69	-0.0073	0.0144	1.34	-0.19	-0.65
o-xylene	0	-0.90	-1.62	0.72	-0.0073	0.0142	1.34	-0.28	-0.62
fluoromethane	0	-0.22	-2.06	1.84	-0.0159	0.0170	0.52	-1.55	1.33
chloromethane	0	-0.56	-1.89	1.33	-0.0089	0.0202	1.18	-0.71	0.15
bromomethane	0	-0.82	-1.79	0.97	-0.0074	0.0208	1.24	-0.55	-0.27
chlorofluoromethane	0	-0.77	-2.65	1.88	-0.0098	0.0262	0.97	-1.68	0.91
dichloromethane	0	-1.36	-2.38	1.02	-0.0052	0.0275	1.10	-1.27	-0.09
dibromomethane	0	-2.11	-2.29	0.18	-0.0042	0.0279	1.11	-1.18	-0.93
chlorodifluoromethane	0	-0.50	-2.25	1.75	-0.0054	0.0334	0.84	-1.41	0.91
chloroform	0	-1.07	-1.88	0.81	-0.0025	0.0332	0.88	-1.00	-0.07
chloroethane	0	-0.63	-1.90	1.27	-0.0097	0.0187	1.17	-0.73	0.10
bromoethane	0	-0.70	-1.83	1.13	-0.0082	0.0193	1.24	-0.59	-0.11
bromoform	0	-1.98	-1.97	-0.01	-0.0020	0.0329	0.90	-1.07	-0.91
tetrafluoromethane	0	3.16	-0.50	3.66	-0.0012	0.0287	1.09	0.59	2.57
difluorodichloromethane	0	1.69	-0.55	2.24	-0.0017	0.0208	1.33	0.78	0.91
fluorotrichloromethane	0	0.82	-0.66	1.48	-0.0022	0.0213	1.32	0.66	0.16
bromotrifluoromethane	0	1.79	-0.60	2.39	-0.0015	0.0280	1.12	0.52	1.27
bromotrichloromethane	0	-0.93	-0.92	-0.01	-0.0007	0.0239	1.26	0.33	-1.26
hexafluoroethane	0	3.94	-0.48	4.42	-0.0012	0.0286	1.10	0.61	3.33
hexachloroethane	0	-1.40	-1.15	-0.25	-0.0027	0.0202	1.34	0.19	-1.59
chloropentafluoroethane	0	2.86	-0.54	3.40	-0.0018	0.0276	1.13	0.59	2.27
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-0.80	2.57	-0.0032	0.0216	1.31	0.51	1.26
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-2.35	2.87	-0.0059	0.0344	0.77	-1.58	2.10
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-2.17	2.04	-0.0039	0.0343	0.81	-1.36	1.23
1-chloro-2,2,2-trifluoroethane	0	0.06	-2.69	2.75	-0.0054	0.0287	1.06	-1.63	1.69
1,1,1,2-tetrachloroethane	0	-1.15	-2.22	1.07	-0.0055	0.0273	1.11	-1.11	-0.04
1,1,1-trichloroethane	0	-0.25	-1.64	1.39	-0.0038	0.0206	1.32	-0.31	0.06
1,1,2-trichloroethane	0	-1.95	-2.73	0.78	-0.0057	0.0287	1.05	-1.69	-0.26

1,1-difluoroethane	0	-0.11	-2.69	2.58	-0.0122	0.0223	0.89	-1.80	1.69
1-bromo-2-chloroethane	0	-1.95	-2.36	0.41	-0.0069	0.0225	1.21	-1.15	-0.80
octafluoropropane	0	4.28	-0.54	4.82	-0.0012	0.0288	1.09	0.54	3.74
2-chloropropane	0	-0.25	-1.88	1.63	-0.0102	0.0177	1.15	-0.73	0.48
1-chloropropane	0	-0.27	-1.89	1.62	-0.0098	0.0181	1.17	-0.72	0.45
1-bromopropane	0	-0.56	-1.83	1.27	-0.0083	0.0187	1.24	-0.59	0.03
2-bromopropane	0	-0.48	-1.82	1.34	-0.0087	0.0184	1.23	-0.60	0.12
2-chlorobutane	0	0.07	-1.76	1.83	-0.0103	0.0172	1.15	-0.61	0.68
1-bromobutane	0	-0.41	-1.87	1.46	-0.0084	0.0187	1.24	-0.64	0.23
1-chloropentane	0	0.07	-1.97	2.04	-0.0099	0.0180	1.16	-0.80	0.87
2-chloropentane	0	0.07	-1.75	1.82	-0.0103	0.0170	1.15	-0.60	0.67
1-bromopentane	0	-0.08	-1.91	1.83	-0.0084	0.0187	1.23	-0.67	0.59
1-bromo-isobutane	0	-0.03	-1.72	1.69	-0.0083	0.0186	1.24	-0.47	0.44
tetrachloroethene	0	0.05	-0.83	0.88	-0.0030	0.0198	1.35	0.52	-0.47
trichloroethene	0	-0.39	-1.32	0.93	-0.0046	0.0290	1.06	-0.26	-0.13
chloroethene	0	-0.59	-1.50	0.91	-0.0069	0.0235	1.19	-0.31	-0.28
E-1,2-dichloroethene	0	-0.76	-1.51	0.75	-0.0045	0.0265	1.15	-0.36	-0.40
Z-1,2-dichloroethene	0	-1.17	-2.12	0.95	-0.0064	0.0272	1.08	-1.03	-0.14
3-chloropropene	0	-0.57	-2.14	1.57	-0.0086	0.0207	1.19	-0.95	0.38
3-bromopropene	0	-0.86	-2.25	1.39	-0.0079	0.0212	1.21	-1.05	0.19
fluorobenzene	0	-0.78	-2.01	1.23	-0.0120	0.0192	0.98	-1.03	0.25
chlorobenzene	0	-1.12	-1.87	0.75	-0.0068	0.0189	1.30	-0.58	-0.54
bromobenzene	0	-1.46	-1.89	0.43	-0.0058	0.0190	1.32	-0.57	-0.89
1,4-dichlorobenzene	0	-1.01	-1.91	0.90	-0.0054	0.0215	1.28	-0.63	-0.38
1,2-dichlorobenzene	0	-1.36	-2.08	0.72	-0.0074	0.0212	1.23	-0.85	-0.51
p-dibromobenzene	0	-2.30	-1.95	-0.35	-0.0046	0.0215	1.29	-0.66	-1.64
chlorotoluene	0	-1.92	-3.12	1.20	-0.0099	0.0201	1.13	-1.99	0.07
o-chlorotoluene	0	-1.15	-1.70	0.55	-0.0071	0.0184	1.29	-0.41	-0.74
bromotoluene	0	-2.37	-3.05	0.68	-0.0084	0.0208	1.19	-1.86	-0.51
p-bromotoluene	0	-1.39	-1.93	0.54	-0.0062	0.0186	1.32	-0.61	-0.78
2,3-dichlorobiphenyl	0	-2.45	-2.88	0.43	-0.0077	0.0206	1.23	-1.66	-0.79
2,2'-dichlorobiphenyl	0	-2.73	-3.16	0.43	-0.0073	0.0190	1.28	-1.88	-0.85
2,2',3'-trichlorobiphenyl	0	-1.99	-3.08	1.09	-0.0075	0.0209	1.23	-1.85	-0.14
1,2-dimethoxyethane	0	-4.84	-2.63	-2.21	-0.0212	0.0136	-0.58	-3.21	-1.63
anisole	0	-2.45	-2.69	0.24	-0.0185	0.0172	0.04	-2.65	0.20

dimethyl ether	0	-1.92	-1.88	-0.04	-0.0225	0.0135	-0.97	-2.85	0.93
diethyl ether	0	-1.76	-1.89	0.13	-0.0233	0.0121	-1.23	-3.12	1.36
isopropyl ether	0	-0.53	-1.76	1.23	-0.0234	0.0123	-1.25	-3.00	2.47
methyl propyl ether	0	-1.66	-1.71	0.05	-0.0223	0.0129	-0.91	-2.63	0.97
methyl isopropyl ether	0	-2.01	-1.72	-0.29	-0.0226	0.0126	-0.97	-2.69	0.68
t-butyl methyl ether	0	-2.21	-1.71	-0.50	-0.0227	0.0122	-1.02	-2.73	0.52
ethyl phenyl ether	0	-2.22	-2.57	0.35	-0.0184	0.0170	0.06	-2.51	0.29
tetrahydrofuran	0	-3.47	-2.16	-1.31	-0.0239	0.0128	-1.43	-3.59	0.12
tetrahydropyran	0	-3.12	-1.93	-1.19	-0.0235	0.0117	-1.27	-3.20	0.08
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-3.09	2.97	-0.0134	0.0237	0.73	-2.36	2.24
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-3.61	3.72	-0.0085	0.0338	0.71	-2.90	3.01
acetaldehyde	0	-3.50	-3.86	0.36	-0.0228	0.0196	-1.13	-4.99	1.49
propanal	0	-3.44	-3.56	0.12	-0.0231	0.0178	-1.20	-4.76	1.32
butanal	0	-3.18	-3.74	0.56	-0.0229	0.0174	-1.15	-4.89	1.71
pentanal	0	-3.03	-3.61	0.58	-0.0230	0.0175	-1.19	-4.80	1.77
octanal	0	-2.29	-3.68	1.39	-0.0232	0.0171	-1.23	-4.92	2.63
benzaldehyde	0	-4.02	-4.22	0.20	-0.0238	0.0204	-1.49	-5.71	1.69
p-hydroxybenzaldehyde	0	-10.48	-7.51	-2.97	-0.0248	0.0573	-4.67	-12.18	1.70
m-hydroxybenzaldehyde	0	-9.51	-7.07	-2.44	-0.0238	0.0564	-4.15	-11.22	1.71
acetone	0	-3.85	-4.13	0.28	-0.0241	0.0180	-1.56	-5.69	1.84
2-butanone	0	-3.64	-3.80	0.16	-0.0243	0.0176	-1.63	-5.44	1.80
2-pentanone	0	-3.53	-3.81	0.28	-0.0244	0.0175	-1.64	-5.46	1.93
3-pentanone	0	-3.41	-3.47	0.06	-0.0239	0.0160	-1.46	-4.94	1.53
2-hexanone	0	-3.29	-3.85	0.56	-0.0244	0.0177	-1.67	-5.52	2.23
2-heptanone	0	-3.04	-3.88	0.84	-0.0244	0.0176	-1.65	-5.54	2.50
4-heptanone	0	-2.93	-3.50	0.57	-0.0241	0.0155	-1.50	-5.00	2.07
2-octanone	0	-2.88	-3.91	1.03	-0.0245	0.0173	-1.67	-5.58	2.70
5-nonanone	0	-2.67	-3.60	0.93	-0.0241	0.0155	-1.53	-5.13	2.46
3,3-dimethylbutanone	0	-2.89	-3.59	0.70	-0.0244	0.0175	-1.64	-5.23	2.34
cyclopentanone	0	-4.68	-4.15	-0.53	-0.0243	0.0165	-1.59	-5.74	1.06
acetophenone	0	-4.58	-4.35	-0.23	-0.0245	0.0190	-1.73	-6.08	1.50
methyl formate	0	-2.78	-3.63	0.85	-0.0218	0.0242	-0.94	-4.58	1.80
ethyl formate	0	-2.65	-3.58	0.93	-0.0221	0.0236	-1.02	-4.60	1.95
methyl acetate	0	-3.32	-3.60	0.28	-0.0233	0.0183	-1.29	-4.89	1.57
ethyl acetate	0	-3.10	-3.58	0.48	-0.0236	0.0179	-1.39	-4.98	1.88

propyl acetate	0	-2.86	-3.59	0.73	-0.0237	0.0179	-1.40	-4.99	2.13
butyl acetate	0	-2.55	-3.62	1.07	-0.0237	0.0176	-1.42	-5.04	2.49
methyl propanoate	0	-2.93	-3.35	0.42	-0.0230	0.0173	-1.18	-4.53	1.60
methyl butanoate	0	-2.83	-3.37	0.54	-0.0231	0.0174	-1.21	-4.59	1.76
methyl pentanoate	0	-2.57	-3.41	0.84	-0.0231	0.0169	-1.21	-4.62	2.05
methyl hexanoate	0	-2.49	-3.43	0.94	-0.0232	0.0169	-1.22	-4.65	2.16
methyl benzoate	0	-3.91	-3.74	-0.17	-0.0231	0.0186	-1.23	-4.97	1.06
hydrogen	0	2.33	-0.12	2.45	-0.0012	0.0127	1.45	1.33	1.00
water	0	-6.31	-5.16	-1.15	-0.0227	0.0490	-2.86	-8.02	1.71
water dimer	0	-11.27	-8.55	-2.72	-0.0264	0.0558	-5.07	-13.62	2.35
hydrogen peroxide	0	-8.58	-5.80	-2.78	-0.0188	0.0543	-2.46	-8.25	-0.33
methyl peroxide	0	-5.28	-4.37	-0.91	-0.0195	0.0527	-2.42	-6.78	1.50
ethyl peroxide	0	-5.32	-4.32	-1.00	-0.0199	0.0519	-2.40	-6.72	1.40
1,4-dioxane	0	-5.05	-3.25	-1.80	-0.0218	0.0153	-0.78	-4.03	-1.02
methanol	0	-5.11	-3.58	-1.53	-0.0230	0.0462	-2.65	-6.23	1.12
ethanol	0	-5.01	-3.31	-1.70	-0.0229	0.0450	-2.49	-5.80	0.79
1-propanol	0	-4.83	-3.30	-1.53	-0.0229	0.0443	-2.44	-5.74	0.91
isopropanol	0	-4.76	-3.22	-1.54	-0.0236	0.0414	-2.42	-5.64	0.88
1-butanol	0	-4.72	-3.34	-1.38	-0.0230	0.0440	-2.43	-5.77	1.05
t-butanol	0	-4.51	-3.04	-1.47	-0.0233	0.0407	-2.26	-5.31	0.80
1-pentanol	0	-4.47	-3.49	-0.98	-0.0235	0.0431	-2.52	-6.01	1.54
1-hexanol	0	-4.36	-3.50	-0.86	-0.0235	0.0426	-2.50	-6.01	1.65
1-heptanol	0	-4.24	-3.51	-0.73	-0.0236	0.0420	-2.47	-5.97	1.73
1-octanol	0	-4.09	-3.61	-0.48	-0.0235	0.0428	-2.51	-6.12	2.03
allyl alcohol	0	-5.08	-3.38	-1.70	-0.0227	0.0443	-2.37	-5.75	0.67
cyclopentanol	0	-5.49	-3.07	-2.42	-0.0236	0.0397	-2.31	-5.38	-0.11
2-methoxyethanol	0	-6.77	-4.61	-2.16	-0.0223	0.0465	-2.46	-7.08	0.31
2,2,2-trifluoroethanol	0	-4.31	-5.74	1.43	-0.0175	0.0548	-2.25	-7.99	3.68
1,1,1-trifluoropropan-2-ol	0	-4.16	-3.73	-0.43	-0.0195	0.0483	-1.89	-5.62	1.46
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-3.97	0.20	-0.0151	0.0564	-2.07	-6.05	2.28
phenol	0	-6.62	-4.40	-2.22	-0.0183	0.0525	-2.11	-6.51	-0.11
p-bromophenol	0	-7.13	-4.83	-2.30	-0.0169	0.0538	-2.01	-6.84	-0.29
o-cresol	0	-5.87	-4.03	-1.84	-0.0176	0.0518	-1.89	-5.92	0.05
m-cresol	0	-5.49	-4.36	-1.13	-0.0187	0.0522	-2.16	-6.52	1.03
p-cresol	0	-6.14	-4.30	-1.84	-0.0189	0.0520	-2.18	-6.48	0.34

1,2-ethanediol	0	-9.30	-5.77	-3.53	-0.0245	0.0504	-3.62	-9.38	0.08
acetic acid	0	-6.70	-4.98	-1.72	-0.0224	0.0556	-3.59	-8.57	1.87
propanoic acid	0	-6.47	-4.72	-1.75	-0.0222	0.0550	-3.44	-8.16	1.69
butanoic acid	0	-6.36	-4.72	-1.64	-0.0222	0.0549	-3.43	-8.15	1.79
pentanoic acid	0	-6.16	-4.76	-1.40	-0.0223	0.0550	-3.47	-8.23	2.07
hexanoic acid	0	-6.21	-4.78	-1.43	-0.0223	0.0544	-3.40	-8.18	1.97
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-8.37	-3.59	-0.0206	0.0556	-3.06	-11.43	-0.53
ammonia	0	-4.29	-3.20	-1.09	-0.0247	0.0281	-2.06	-5.25	0.96
methylamine	0	-4.56	-2.54	-2.02	-0.0243	0.0263	-1.85	-4.39	-0.17
ethylamine	0	-4.50	-2.58	-1.92	-0.0245	0.0252	-1.88	-4.46	-0.04
butylamine	0	-4.29	-2.64	-1.65	-0.0247	0.0252	-1.95	-4.58	0.29
propylamine	0	-4.39	-2.60	-1.79	-0.0247	0.0252	-1.93	-4.53	0.14
pentylamine	0	-4.10	-2.66	-1.44	-0.0248	0.0246	-1.96	-4.63	0.53
dimethylamine	0	-4.29	-1.85	-2.44	-0.0232	0.0261	-1.44	-3.29	-1.00
diethylamine	0	-4.07	-1.76	-2.31	-0.0231	0.0240	-1.34	-3.10	-0.97
dipropylamine	0	-3.66	-1.80	-1.86	-0.0229	0.0240	-1.29	-3.10	-0.56
trimethylamine	0	-3.23	-1.15	-2.08	-0.0217	0.0115	-0.70	-1.85	-1.38
azetidine	0	-5.56	-2.05	-3.51	-0.0243	0.0248	-1.77	-3.82	-1.74
pyrrolidine	0	-5.48	-2.22	-3.26	-0.0243	0.0247	-1.80	-4.02	-1.46
piperidine	0	-5.11	-1.54	-3.57	-0.0226	0.0254	-1.22	-2.76	-2.35
2-methoxyethanamine	0	-6.55	-4.05	-2.50	-0.0238	0.0272	-1.67	-5.72	-0.83
1,2-ethanediamine	0	-9.72	-4.96	-4.76	-0.0238	0.0267	-1.68	-6.64	-3.08
nitromethane	0	-3.95	-5.22	1.27	-0.0178	0.0272	-0.07	-5.30	1.35
nitroethane	0	-3.71	-4.91	1.20	-0.0185	0.0246	-0.12	-5.03	1.32
1-nitropropane	0	-3.34	-4.83	1.49	-0.0185	0.0240	-0.12	-4.95	1.61
2-nitropropane	0	-3.14	-4.45	1.31	-0.0188	0.0227	-0.14	-4.59	1.45
1-nitrobutane	0	-3.08	-4.85	1.77	-0.0186	0.0239	-0.13	-4.98	1.90
nitrobenzene	0	-4.12	-4.49	0.37	-0.0185	0.0222	-0.07	-4.56	0.44
2-methyl-1-nitrobenzene	0	-3.59	-4.27	0.68	-0.0193	0.0210	-0.23	-4.50	0.91
pyridine	0	-4.70	-3.10	-1.60	-0.0246	0.0204	-1.79	-4.89	0.19
2-methylpyridine	0	-4.63	-2.77	-1.86	-0.0246	0.0193	-1.75	-4.52	-0.11
3-methylpyridine	0	-4.77	-3.16	-1.61	-0.0251	0.0191	-1.95	-5.11	0.34
4-methylpyridine	0	-4.94	-3.26	-1.68	-0.0253	0.0181	-2.02	-5.28	0.34
4-ethylpyridine	0	-4.74	-3.27	-1.47	-0.0254	0.0180	-2.05	-5.32	0.58
2,4-dimethylpyridine	0	-4.86	-2.92	-1.94	-0.0252	0.0170	-1.96	-4.88	0.02

2,5-dimethylpyridine	0	-4.72	-2.81	-1.91	-0.0249	0.0182	-1.87	-4.68	-0.04
2,6-dimethylpyridine	0	-4.60	-2.46	-2.14	-0.0244	0.0187	-1.67	-4.13	-0.47
3,4-dimethylpyridine	0	-5.22	-3.41	-1.81	-0.0258	0.0175	-2.17	-5.58	0.36
3,5-dimethylpyridine	0	-4.84	-3.22	-1.62	-0.0256	0.0182	-2.10	-5.32	0.48
aniline	0	-5.49	-4.15	-1.35	-0.0180	0.0352	-0.48	-4.62	-0.87
N-methylaniline	0	-4.68	-3.36	-1.32	-0.0154	0.0347	0.00	-3.36	-1.32
2-methylaniline	0	-5.56	-3.78	-1.78	-0.0182	0.0338	-0.45	-4.22	-1.34
3-methylaniline	0	-5.67	-4.04	-1.63	-0.0182	0.0342	-0.48	-4.52	-1.15
4-methylaniline	0	-5.55	-3.97	-1.58	-0.0187	0.0339	-0.56	-4.53	-1.02
N-ethylaniline	0	-4.62	-3.26	-1.36	-0.0135	0.0351	0.23	-3.03	-1.59
3-aminoaniline	0	-9.92	-6.58	-3.34	-0.0184	0.0342	-0.52	-7.10	-2.82
N,N-dimethylaniline	0	-3.58	-2.60	-0.98	-0.0123	0.0158	1.00	-1.60	-1.98
piperazine	0	-7.40	-2.91	-4.49	-0.0223	0.0259	-1.17	-4.08	-3.32
N-methylpiperazine	0	-7.77	-2.32	-5.45	-0.0222	0.0263	-1.14	-3.46	-4.31
N,N'-dimethylpiperazine	0	-7.58	-1.69	-5.89	-0.0207	0.0116	-0.42	-2.11	-5.47
1-methylthymine	0	-10.40	-8.90	-1.50	-0.0254	0.0475	-3.65	-12.56	2.16
9-methyladenine	0	-13.60	-7.35	-6.25	-0.0239	0.0423	-2.59	-9.94	-3.66
acetamide	0	-9.71	-6.98	-2.73	-0.0268	0.0439	-3.87	-10.85	1.14
E-N-methylacetamide	0	-10.00	-6.44	-3.56	-0.0280	0.0377	-3.92	-10.36	0.36
Z-N-methylacetamide	0	-10.00	-6.06	-3.94	-0.0281	0.0430	-4.36	-10.41	0.41
benzamide	0	-10.90	-6.85	-4.05	-0.0259	0.0430	-3.43	-10.28	-0.62
2,6-dichlorothiobenzamide	0	-10.81	-7.78	-3.03	-0.0166	0.0515	-1.66	-9.44	-1.37
urea	0	-13.80	-8.50	-5.30	-0.0263	0.0424	-3.52	-12.02	-1.78
1,1-dimethyl-3-phenylurea	0	-9.63	-6.71	-2.92	-0.0260	0.0378	-3.04	-9.76	0.13
hydrazine	0	-6.26	-4.32	-1.94	-0.0229	0.0284	-1.43	-5.75	-0.51
methylhydrazine	0	-5.31	-3.94	-1.37	-0.0229	0.0282	-1.41	-5.36	0.05
1,1-dimethylhydrazine	0	-4.48	-3.02	-1.46	-0.0229	0.0282	-1.44	-4.46	-0.02
2-methylpyrazine	0	-5.57	-3.23	-2.34	-0.0220	0.0197	-0.91	-4.15	-1.42
2-ethylpyrazine	0	-5.51	-2.96	-2.55	-0.0221	0.0196	-0.93	-3.89	-1.62
morpholine	0	-7.17	-3.22	-3.95	-0.0231	0.0278	-1.47	-4.69	-2.48
N-methylmorpholine	0	-6.34	-2.51	-3.83	-0.0228	0.0134	-1.08	-3.59	-2.75
acetonitrile	0	-3.89	-5.39	1.50	-0.0240	0.0251	-1.68	-7.08	3.19
butanonitrile	0	-3.64	-4.87	1.23	-0.0241	0.0225	-1.65	-6.52	2.88
propionitrile	0	-3.85	-5.08	1.23	-0.0242	0.0228	-1.67	-6.76	2.91
benzonitrile	0	-4.10	-4.96	0.86	-0.0237	0.0232	-1.54	-6.50	2.40

2,6-dichlorobenzonitrile	0	-5.22	-5.23	0.01	-0.0230	0.0258	-1.36	-6.59	1.37
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-6.00	-3.00	-0.0227	0.0469	-2.64	-8.64	-0.36
trimethylphosphate	0	-8.70	-6.30	-2.40	-0.0263	0.0192	-2.41	-8.70	0.00
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-5.53	-1.08	-0.0232	0.0271	-1.47	-6.99	0.38
phosphine	0	0.60	-0.44	1.04	-0.0085	0.0139	1.29	0.86	-0.26
hydrogen sulfide	0	-0.70	-1.62	0.92	-0.0100	0.0253	0.99	-0.63	-0.07
dimethyl sulfide	0	-1.54	-1.85	0.31	-0.0140	0.0165	0.79	-1.06	-0.48
diethyl sulfide	0	-1.43	-1.71	0.28	-0.0146	0.0131	0.76	-0.94	-0.49
dipropyl sulfide	0	-1.27	-1.79	0.52	-0.0148	0.0126	0.74	-1.05	-0.22
bis(2-chloroethyl)sulfide	0	-3.92	-3.71	-0.21	-0.0101	0.0207	1.10	-2.61	-1.31
dimethyl disulfide	0	-1.83	-2.15	0.32	-0.0109	0.0184	1.08	-1.07	-0.76
diethyl disulfide	0	-1.63	-1.91	0.28	-0.0112	0.0166	1.09	-0.82	-0.81
methanethiol	0	-1.24	-1.77	0.53	-0.0123	0.0212	0.90	-0.87	-0.37
ethanethiol	0	-1.30	-1.76	0.46	-0.0126	0.0202	0.89	-0.86	-0.44
1-propanethiol	0	-1.05	-1.80	0.75	-0.0128	0.0202	0.88	-0.92	-0.13
thiophene	0	-1.42	-1.87	0.45	-0.0066	0.0219	1.24	-0.63	-0.79
thiophenol	0	-2.55	-2.58	0.03	-0.0093	0.0246	1.05	-1.53	-1.02
thioanisole	0	-2.73	-2.72	-0.01	-0.0110	0.0194	1.06	-1.66	-1.07
tetramethylsilane	0	3.04	-0.60	3.64	-0.0039	0.0109	1.45	0.85	2.19
acetylene	-1	-76.50	-61.01	-15.49	-0.0446	0.0040	-16.04	-77.05	0.55
acetonitrile	-1	-66.60	-56.45	-10.15	-0.0445	-0.0061	-15.93	-72.38	5.78
cyanamide	-1	-72.20	-59.56	-12.64	-0.0450	0.0062	-16.49	-76.05	3.85
aniline	-1	-62.90	-50.83	-12.07	-0.0438	0.0007	-15.18	-66.01	3.11
diphenylamine	-1	-54.60	-44.17	-10.43	-0.0374	0.0041	-9.07	-53.24	-1.36
hydrogen cyanide	-1	-70.20	-61.80	-8.40	-0.0439	-0.0337	-15.31	-77.10	6.90
formic acid	-1	-76.20	-60.91	-15.29	-0.0444	-0.0127	-15.86	-76.77	0.57
acetic acid	-1	-77.60	-59.61	-17.99	-0.0455	-0.0009	-17.08	-76.69	-0.91
propanoic acid	-1	-76.20	-57.74	-18.46	-0.0454	0.0017	-17.00	-74.74	-1.46
hexanoic acid	-1	-74.60	-56.71	-17.89	-0.0454	0.0078	-16.98	-73.69	-0.91
acrylic acid	-1	-74.00	-58.36	-15.64	-0.0451	0.0060	-16.60	-74.97	0.97
pyruvic acid	-1	-68.50	-57.20	-11.30	-0.0431	0.0074	-14.42	-71.62	3.12
benzoic acid	-1	-71.20	-55.49	-15.71	-0.0445	0.0097	-15.90	-71.38	0.18
methanol	-1	-95.00	-62.15	-32.85	-0.0542	-0.0188	-29.31	-91.46	-3.54
ethanol	-1	-90.70	-58.45	-32.25	-0.0535	-0.0056	-28.19	-86.64	-4.06
1-propanol	-1	-88.30	-57.80	-30.50	-0.0537	0.0004	-28.58	-86.37	-1.93

isopropanol	-1	-86.30	-55.72	-30.58	-0.0531	-0.0049	-27.58	-83.30	-3.00
2-butanol	-1	-84.20	-53.36	-30.84	-0.0521	-0.0040	-26.08	-79.43	-4.77
t-butanol	-1	-82.30	-53.63	-28.67	-0.0529	-0.0041	-27.29	-80.92	-1.38
allyl alcohol	-1	-86.60	-57.60	-29.00	-0.0528	0.0010	-27.05	-84.65	-1.95
benzyl alcohol	-1	-85.10	-53.85	-31.25	-0.0516	0.0066	-25.32	-79.17	-5.93
2-methoxyethanol	-1	-89.40	-58.72	-30.68	-0.0532	0.0054	-27.81	-86.53	-2.87
phenol	-1	-71.90	-52.79	-19.11	-0.0469	0.0014	-18.82	-71.61	-0.29
2-methylphenol	-1	-70.20	-51.01	-19.19	-0.0467	0.0006	-18.49	-69.50	-0.70
3-methylphenol	-1	-71.10	-52.39	-18.71	-0.0471	0.0042	-19.06	-71.45	0.35
4-methylphenol	-1	-72.00	-52.37	-19.63	-0.0475	0.0036	-19.54	-71.90	-0.10
1,2-ethanediol	-1	-85.30	-61.08	-24.22	-0.0535	0.0332	-28.78	-89.86	4.56
3-hydroxyphenol	-1	-73.80	-53.66	-20.14	-0.0462	0.0382	-18.80	-72.47	-1.33
4-hydroxyphenol	-1	-77.60	-54.85	-22.75	-0.0476	0.0373	-20.55	-75.40	-2.20
methyl hydroperoxide	-1	-93.20	-63.56	-29.64	-0.0515	-0.0038	-25.08	-88.64	-4.56
ethyl hydroperoxide	-1	-89.20	-62.67	-26.53	-0.0517	0.0028	-25.35	-88.02	-1.18
acetaldehyde	-1	-76.50	-57.73	-18.77	-0.0481	-0.0074	-20.38	-78.11	1.61
acetone	-1	-76.20	-56.01	-20.19	-0.0483	-0.0027	-20.57	-76.58	0.38
3-pentanone	-1	-73.70	-51.56	-22.14	-0.0476	-0.0005	-19.70	-71.27	-2.43
water	-1	-104.70	-70.80	-33.90	-0.0574	-0.0114	-34.99	-105.80	1.10
hydrogen peroxide	-1	-97.30	-69.09	-28.21	-0.0521	0.0166	-26.06	-95.15	-2.15
hydroperoxyl radical	-1	-83.30	-67.40	-15.90	-0.0480	-0.0411	-20.18	-87.58	4.28
2-nitrophenol	-1	-60.10	-50.81	-9.29	-0.0419	0.0082	-13.12	-63.93	3.83
3-nitrophenol	-1	-61.90	-47.91	-13.99	-0.0435	0.0112	-14.81	-62.72	0.82
4-nitrophenol	-1	-57.80	-46.64	-11.16	-0.0396	0.0079	-10.90	-57.54	-0.26
nitromethane	-1	-76.50	-58.64	-17.86	-0.0438	0.0004	-15.10	-73.74	-2.76
4-nitroaniline	-1	-57.40	-46.34	-11.06	-0.0370	0.0078	-8.75	-55.09	-2.31
acetamide	-1	-80.20	-57.24	-22.96	-0.0460	-0.0022	-17.67	-74.90	-5.30
methanethiol	-1	-73.80	-56.49	-17.31	-0.0364	-0.0048	-8.20	-64.69	-9.11
ethanethiol	-1	-71.80	-54.08	-17.72	-0.0362	-0.0016	-8.08	-62.17	-9.63
1-propanethiol	-1	-70.50	-53.75	-16.75	-0.0363	0.0036	-8.16	-61.91	-8.59
thiophenol	-1	-63.40	-50.09	-13.31	-0.0330	0.0058	-5.86	-55.95	-7.45
hydrogen sulfide	-1	-72.10	-58.24	-13.86	-0.0359	-0.0107	-7.85	-66.10	-6.00
dimethyl sulfoxide	-1	-67.70	-53.77	-13.93	-0.0451	0.0019	-16.58	-70.36	2.66
hydrofluoric acid	-1	-104.40	-77.06	-27.34	-0.0598	-0.0598	-39.49	-116.55	12.15
hydrochloric acid	-1	-74.50	-62.34	-12.16	-0.0382	-0.0382	-9.72	-72.06	-2.44

hydrobromic acid	-1	-68.30	-58.78	-9.52	-0.0337	-0.0337	-6.30	-65.08	-3.22
chloroform	-1	-54.10	-48.46	-5.64	-0.0313	-0.0117	-4.80	-53.27	-0.83
trifluoroacetic acid	-1	-59.30	-54.31	-4.99	-0.0407	0.0108	-12.01	-66.32	7.02
chloroacetic acid	-1	-69.70	-55.09	-14.61	-0.0424	0.0064	-13.64	-68.72	-0.98
dichloroacetic acid	-1	-62.30	-52.24	-10.06	-0.0403	0.0113	-11.61	-63.85	1.55
2,2,2-trifluoroethanol	-1	-77.50	-56.10	-21.40	-0.0506	-0.0023	-23.79	-79.88	2.38
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-51.84	-13.66	-0.0473	0.0025	-19.26	-71.10	5.60
2-chlorophenol	-1	-66.10	-50.63	-15.47	-0.0450	0.0052	-16.45	-67.08	0.98
4-chlorophenol	-1	-66.00	-49.27	-16.73	-0.0454	0.0053	-16.95	-66.22	0.22
methylamine	1	-76.40	-69.39	-7.01	0.0243	0.0817	-6.74	-76.13	-0.27
n-propylamine	1	-71.50	-64.03	-7.47	0.0065	0.0805	-6.38	-70.41	-1.09
isopropylamine	1	-69.60	-62.22	-7.38	0.0112	0.0779	-5.67	-67.89	-1.71
tert-butylamine	1	-67.30	-59.39	-7.91	0.0111	0.0757	-5.10	-64.49	-2.81
cyclohexanamine	1	-68.70	-59.14	-9.56	0.0071	0.0770	-5.42	-64.57	-4.13
allylamine	1	-72.00	-64.15	-7.85	-0.0001	0.0811	-6.57	-70.72	-1.28
dimethylamine	1	-68.60	-62.13	-6.47	0.0220	0.0768	-5.40	-67.53	-1.07
diethylamine	1	-63.40	-55.80	-7.60	0.0110	0.0703	-3.83	-59.64	-3.76
di-n-propylamine	1	-60.50	-53.43	-7.07	0.0071	0.0702	-3.80	-57.22	-3.28
diallylamine	1	-61.60	-53.82	-7.78	0.0010	0.0717	-4.14	-57.96	-3.64
trimethylamine	1	-61.10	-56.12	-4.98	0.0212	0.0729	-4.43	-60.55	-0.55
triethylamine	1	-54.60	-48.49	-6.11	0.0099	0.0603	-1.93	-50.42	-4.18
aniline	1	-72.40	-62.52	-9.88	0.0022	0.0825	-6.96	-69.49	-2.91
2-methylaniline	1	-70.30	-60.14	-10.16	0.0012	0.0802	-6.30	-66.44	-3.86
3-methylaniline	1	-69.60	-60.88	-8.72	0.0012	0.0816	-6.70	-67.58	-2.02
4-methylaniline	1	-69.80	-60.72	-9.08	0.0019	0.0814	-6.63	-67.35	-2.45
3-aminoaniline	1	-65.80	-61.72	-4.08	-0.0080	0.0807	-6.58	-68.29	2.49
N-methylaniline	1	-62.60	-55.81	-6.79	0.0015	0.0761	-5.20	-61.01	-1.59
N-ethylaniline	1	-62.20	-52.89	-9.31	0.0013	0.0730	-4.44	-57.33	-4.87
N,N-dimethylaniline	1	-57.20	-50.42	-6.78	0.0014	0.0701	-3.78	-54.20	-3.00
4-methyl-N,N-dimethylaniline	1	-55.90	-48.99	-6.91	0.0015	0.0692	-3.58	-52.57	-3.33
N,N-diethylaniline	1	-54.00	-46.31	-7.69	0.0002	0.0631	-2.40	-48.71	-5.29
1-aminonaphthalene	1	-67.40	-58.77	-8.63	0.0003	0.0827	-7.04	-65.80	-1.60
aziridine	1	-70.90	-63.90	-7.00	0.0239	0.0811	-6.56	-70.46	-0.44
azetidine	1	-67.70	-60.38	-7.32	0.0160	0.0755	-5.06	-65.44	-2.26
pyrrolidine	1	-66.00	-57.97	-8.03	0.0118	0.0743	-4.74	-62.71	-3.29

piperidine	1	-64.20	-56.04	-8.16	0.0115	0.0745	-4.81	-60.85	-3.35
azacycloheptane	1	-63.30	-54.37	-8.93	0.0101	0.0745	-4.80	-59.17	-4.13
pyrrole	1	-61.40	-56.48	-4.92	0.0135	0.0780	-5.71	-62.19	0.79
pyridine	1	-61.10	-54.72	-6.38	0.0152	0.0789	-5.95	-60.67	-0.43
quinoline	1	-56.00	-48.81	-7.19	0.0056	0.0728	-4.39	-53.20	-2.80
piperazine	1	-66.00	-57.46	-8.54	-0.0108	0.0750	-5.21	-62.67	-3.33
acetonitrile	1	-75.30	-63.81	-11.49	0.0296	0.1157	-21.05	-84.86	9.56
ammonia	1	-85.20	-78.50	-6.70	0.0541	0.0881	-8.74	-87.24	2.04
hydrazine	1	-84.60	-75.31	-9.29	-0.0015	0.0861	-8.10	-83.41	-1.19
methanol	1	-93.00	-74.44	-18.56	0.0175	0.1176	-22.18	-96.63	3.63
ethanol	1	-88.40	-68.83	-19.57	0.0135	0.1133	-19.76	-88.58	0.18
dimethyl ether	1	-79.70	-63.30	-16.40	0.0145	0.1087	-17.34	-80.64	0.94
diethyl ether	1	-71.50	-55.29	-16.21	0.0101	0.0943	-10.99	-66.28	-5.22
acetone	1	-77.10	-60.05	-17.05	0.0087	0.0967	-11.90	-71.95	-5.15
acetophenone	1	-64.50	-49.42	-15.08	0.0046	0.0812	-6.59	-56.02	-8.48
water	1	-110.30	-89.69	-20.61	0.0221	0.1304	-30.40	-120.09	9.79
4-methoxyaniline	1	-71.20	-60.74	-10.46	-0.0120	0.0814	-7.03	-67.77	-3.43
4-nitroaniline	1	-75.90	-72.55	-3.35	-0.0124	0.0876	-8.99	-81.54	5.64
morpholine	1	-69.60	-60.91	-8.69	-0.0103	0.0774	-5.80	-66.70	-2.90
acetamide	1	-73.90	-64.31	-9.59	0.0041	0.0922	-10.19	-74.49	0.59
benzamide	1	-67.20	-56.19	-11.01	0.0033	0.0891	-9.07	-65.26	-1.94
dimethyl sulfide	1	-64.50	-57.27	-7.23	0.0197	0.0583	-1.60	-58.87	-5.63
dimethyl sulfoxide	1	-67.70	-57.45	-10.25	0.0016	0.0888	-8.97	-66.41	-1.29
3-chloroaniline	1	-74.70	-64.67	-10.03	-0.0025	0.0850	-7.73	-72.40	-2.30
4-chloroaniline	1	-74.10	-64.91	-9.19	-0.0012	0.0844	-7.55	-72.46	-1.64
PEARSON			0.99					1.00	

Table S 6-2

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/G3large method for the cavity surface with constant density = 0.001 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.26	2.26	0.0002	0.0189	2.11	1.85	0.15
ethane	0	1.83	-0.25	2.08	-0.0002	0.0165	2.11	1.86	-0.03
n-propane	0	1.96	-0.31	2.27	-0.0003	0.0163	2.11	1.80	0.16
n-butane	0	2.08	-0.37	2.45	-0.0004	0.0164	2.11	1.75	0.33
n-pentane	0	2.33	-0.42	2.75	-0.0004	0.0163	2.11	1.70	0.63
n-hexane	0	2.49	-0.47	2.96	-0.0005	0.0163	2.11	1.65	0.84
n-heptane	0	2.62	-0.52	3.14	-0.0005	0.0158	2.11	1.60	1.02
n-octane	0	2.89	-0.56	3.45	-0.0005	0.0157	2.11	1.56	1.33
2-methylpropane	0	2.32	-0.41	2.73	-0.0003	0.0163	2.11	1.70	0.62
2,2-dimethylpropane	0	2.50	-0.53	3.03	-0.0002	0.0163	2.11	1.58	0.92
2-methylpentane	0	2.52	-0.49	3.01	-0.0006	0.0161	2.11	1.63	0.89
2,4-dimethylpentane	0	2.88	-0.59	3.47	-0.0005	0.0166	2.11	1.52	1.36
2,2,4-trimethylpentane	0	2.85	-0.69	3.54	-0.0015	0.0170	2.11	1.42	1.43
cyclopropane	0	0.75	-0.96	1.71	-0.0081	0.0204	2.07	1.11	-0.36
cyclopentane	0	1.20	-0.35	1.55	-0.0009	0.0158	2.11	1.76	-0.56
cyclohexane	0	1.23	-0.32	1.55	-0.0005	0.0148	2.12	1.80	-0.57
methylcyclohexane	0	1.71	-0.41	2.12	-0.0006	0.0159	2.11	1.71	0.00
cis-1,2-dimethylcyclohexane	0	1.58	-0.48	2.06	-0.0007	0.0162	2.11	1.63	-0.05
ethene	0	1.27	-1.13	2.40	-0.0099	0.0240	2.03	0.89	0.38
propene	0	1.27	-1.15	2.42	-0.0110	0.0219	2.01	0.87	0.40
1-butene	0	1.38	-1.14	2.52	-0.0113	0.0213	2.00	0.87	0.51
1-pentene	0	1.66	-1.19	2.85	-0.0114	0.0211	2.00	0.81	0.85
E-2-pentene	0	1.34	-1.02	2.36	-0.0112	0.0198	2.01	0.99	0.35
1-hexene	0	1.68	-1.29	2.97	-0.0111	0.0214	2.01	0.72	0.96
2-methylpropene	0	1.16	-1.20	2.36	-0.0117	0.0201	2.00	0.80	0.36
s-trans-1,3-butadiene	0	0.61	-1.84	2.45	-0.0081	0.0245	2.06	0.21	0.40
cyclopentene	0	0.56	-0.95	1.51	-0.0115	0.0226	1.99	1.04	-0.48
ethyne	0	-0.01	-3.46	3.45	-0.0107	0.0514	1.67	-1.79	1.78
propyne	0	-0.31	-3.03	2.72	-0.0132	0.0461	1.70	-1.34	1.03
1-butyne	0	-0.16	-2.92	2.76	-0.0135	0.0460	1.68	-1.23	1.07
1-pentyne	0	0.01	-2.79	2.80	-0.0135	0.0456	1.69	-1.10	1.11
1-hexyne	0	0.29	-3.04	3.33	-0.0137	0.0452	1.69	-1.35	1.64

butenyne	0	0.04	-3.14	3.18	-0.0121	0.0486	1.69	-1.45	1.49
benzene	0	-0.87	-2.26	1.39	-0.0042	0.0247	2.08	-0.17	-0.70
ethylbenzene	0	-0.80	-2.26	1.46	-0.0054	0.0238	2.08	-0.17	-0.63
naphthalene	0	-2.39	-3.15	0.76	-0.0048	0.0251	2.08	-1.06	-1.33
anthracene	0	-4.23	-4.01	-0.22	-0.0050	0.0250	2.08	-1.92	-2.31
toluene	0	-0.89	-2.23	1.34	-0.0054	0.0239	2.08	-0.15	-0.74
p-xylene	0	-0.81	-2.16	1.35	-0.0063	0.0223	2.08	-0.08	-0.73
m-xylene	0	-0.84	-2.19	1.35	-0.0066	0.0232	2.08	-0.11	-0.73
o-xylene	0	-0.90	-2.29	1.39	-0.0065	0.0230	2.08	-0.21	-0.69
fluoromethane	0	-0.22	-2.65	2.43	-0.0179	0.0261	1.64	-1.01	0.79
chloromethane	0	-0.56	-2.49	1.93	-0.0091	0.0302	2.01	-0.48	-0.08
bromomethane	0	-0.82	-2.38	1.56	-0.0071	0.0310	2.03	-0.35	-0.47
chlorofluoromethane	0	-0.77	-3.54	2.77	-0.0106	0.0381	1.90	-1.64	0.87
dichloromethane	0	-1.36	-3.26	1.90	-0.0046	0.0400	1.95	-1.31	-0.05
dibromomethane	0	-2.11	-3.18	1.07	-0.0031	0.0403	1.95	-1.23	-0.88
chlorodifluoromethane	0	-0.50	-3.10	2.60	-0.0051	0.0475	1.83	-1.28	0.78
chloroform	0	-1.07	-2.72	1.65	-0.0010	0.0476	1.83	-0.89	-0.18
chloroethane	0	-0.63	-2.51	1.88	-0.0101	0.0283	2.00	-0.51	-0.12
bromoethane	0	-0.70	-2.43	1.73	-0.0080	0.0290	2.03	-0.39	-0.31
bromoform	0	-1.98	-2.91	0.93	-0.0002	0.0472	1.84	-1.07	-0.91
tetrafluoromethane	0	3.16	-0.86	4.02	-0.0002	0.0422	1.93	1.06	2.10
difluorodichloromethane	0	1.69	-0.94	2.63	-0.0007	0.0308	2.05	1.12	0.57
fluorotrichloromethane	0	0.82	-1.08	1.90	-0.0013	0.0316	2.05	0.97	-0.15
bromotrifluoromethane	0	1.79	-1.03	2.82	-0.0005	0.0415	1.94	0.90	0.89
bromotrichloromethane	0	-0.93	-1.46	0.53	0.0013	0.0363	2.00	0.55	-1.48
hexafluoroethane	0	3.94	-0.92	4.86	-0.0002	0.0423	1.92	1.00	2.94
hexachloroethane	0	-1.40	-1.80	0.40	-0.0013	0.0302	2.06	0.26	-1.66
chloropentafluoroethane	0	2.86	-0.98	3.84	-0.0009	0.0406	1.95	0.97	1.89
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-1.28	3.05	-0.0026	0.0320	2.04	0.77	1.00
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-3.37	3.89	-0.0062	0.0488	1.79	-1.58	2.10
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-3.17	3.04	-0.0033	0.0488	1.80	-1.37	1.24
1-chloro-2,2,2-trifluoroethane	0	0.06	-3.71	3.77	-0.0050	0.0410	1.94	-1.77	1.83
1,1,1,2-tetrachloroethane	0	-1.15	-3.22	2.07	-0.0045	0.0396	1.96	-1.26	0.11
1,1,1-trichloroethane	0	-0.25	-2.29	2.04	-0.0031	0.0306	2.05	-0.24	-0.01
1,1,2-trichloroethane	0	-1.95	-3.93	1.98	-0.0058	0.0417	1.92	-2.01	0.06

1,1-difluoroethane	0	-0.11	-3.53	3.42	-0.0134	0.0331	1.87	-1.66	1.55
1-bromo-2-chloroethane	0	-1.95	-3.38	1.43	-0.0070	0.0333	2.01	-1.37	-0.58
octafluoropropane	0	4.28	-1.06	5.34	-0.0002	0.0421	1.93	0.87	3.41
2-chloropropane	0	-0.25	-2.52	2.27	-0.0108	0.0271	1.99	-0.53	0.28
1-chloropropane	0	-0.27	-2.52	2.25	-0.0102	0.0276	2.00	-0.52	0.25
1-bromopropane	0	-0.56	-2.45	1.89	-0.0082	0.0284	2.04	-0.42	-0.14
2-bromopropane	0	-0.48	-2.45	1.97	-0.0087	0.0280	2.03	-0.42	-0.06
2-chlorobutane	0	0.07	-2.38	2.45	-0.0109	0.0264	1.99	-0.39	0.46
1-bromobutane	0	-0.41	-2.51	2.10	-0.0083	0.0283	2.03	-0.48	0.07
1-chloropentane	0	0.07	-2.64	2.71	-0.0104	0.0275	2.00	-0.64	0.71
2-chloropentane	0	0.07	-2.40	2.47	-0.0109	0.0263	1.99	-0.41	0.48
1-bromopentane	0	-0.08	-2.56	2.48	-0.0083	0.0284	2.03	-0.53	0.45
1-bromo-isobutane	0	-0.03	-2.34	2.31	-0.0081	0.0283	2.04	-0.30	0.27
tetrachloroethene	0	0.05	-1.33	1.38	-0.0017	0.0295	2.06	0.73	-0.68
trichloroethene	0	-0.39	-1.94	1.55	-0.0032	0.0422	1.93	-0.02	-0.37
chloroethene	0	-0.59	-2.06	1.47	-0.0068	0.0348	2.00	-0.06	-0.53
E-1,2-dichloroethene	0	-0.76	-2.21	1.45	-0.0043	0.0389	1.97	-0.24	-0.52
Z-1,2-dichloroethene	0	-1.17	-2.86	1.69	-0.0050	0.0398	1.95	-0.91	-0.26
3-chloropropene	0	-0.57	-2.94	2.37	-0.0087	0.0310	2.01	-0.93	0.36
3-bromopropene	0	-0.86	-3.08	2.22	-0.0076	0.0316	2.02	-1.06	0.20
fluorobenzene	0	-0.78	-2.74	1.96	-0.0132	0.0295	1.90	-0.84	0.06
chlorobenzene	0	-1.12	-2.56	1.44	-0.0068	0.0290	2.05	-0.52	-0.60
bromobenzene	0	-1.46	-2.60	1.14	-0.0053	0.0293	2.06	-0.55	-0.91
1,4-dichlorobenzene	0	-1.01	-2.70	1.69	-0.0052	0.0322	2.03	-0.67	-0.34
1,2-dichlorobenzene	0	-1.36	-2.83	1.47	-0.0068	0.0318	2.03	-0.80	-0.56
p-dibromobenzene	0	-2.30	-2.79	0.49	-0.0041	0.0320	2.04	-0.75	-1.55
chlorotoluene	0	-1.92	-4.22	2.30	-0.0101	0.0302	1.99	-2.23	0.31
o-chlorotoluene	0	-1.15	-2.39	1.24	-0.0073	0.0285	2.05	-0.34	-0.81
bromotoluene	0	-2.37	-4.14	1.77	-0.0082	0.0312	2.02	-2.13	-0.24
p-bromotoluene	0	-1.39	-2.65	1.26	-0.0058	0.0286	2.06	-0.59	-0.80
2,3-dichlorobiphenyl	0	-2.45	-4.00	1.55	-0.0069	0.0311	2.03	-1.97	-0.48
2,2'-dichlorobiphenyl	0	-2.73	-4.34	1.61	-0.0073	0.0290	2.04	-2.30	-0.43
2,2',3'-trichlorobiphenyl	0	-1.99	-4.28	2.29	-0.0069	0.0315	2.03	-2.26	0.27
1,2-dimethoxyethane	0	-4.84	-3.81	-1.03	-0.0253	0.0217	0.71	-3.09	-1.75
anisole	0	-2.45	-3.71	1.26	-0.0220	0.0266	1.21	-2.51	0.06

dimethyl ether	0	-1.92	-2.57	0.65	-0.0265	0.0218	0.48	-2.09	0.17
diethyl ether	0	-1.76	-2.67	0.91	-0.0277	0.0198	0.24	-2.43	0.67
isopropyl ether	0	-0.53	-2.58	2.05	-0.0279	0.0197	0.19	-2.39	1.86
methyl propyl ether	0	-1.66	-2.44	0.78	-0.0264	0.0210	0.50	-1.94	0.28
methyl isopropyl ether	0	-2.01	-2.47	0.46	-0.0268	0.0207	0.43	-2.04	0.03
t-butyl methyl ether	0	-2.21	-2.49	0.28	-0.0270	0.0201	0.38	-2.11	-0.10
ethyl phenyl ether	0	-2.22	-3.61	1.39	-0.0220	0.0263	1.20	-2.41	0.19
tetrahydrofuran	0	-3.47	-2.92	-0.55	-0.0282	0.0209	0.12	-2.81	-0.66
tetrahydropyran	0	-3.12	-2.67	-0.45	-0.0279	0.0194	0.20	-2.47	-0.65
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-4.34	4.22	-0.0156	0.0348	1.73	-2.61	2.49
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-5.16	5.27	-0.0098	0.0485	1.75	-3.41	3.52
acetaldehyde	0	-3.50	-5.01	1.51	-0.0269	0.0297	0.37	-4.65	1.15
propanal	0	-3.44	-4.68	1.24	-0.0272	0.0282	0.31	-4.37	0.93
butanal	0	-3.18	-4.89	1.71	-0.0270	0.0276	0.35	-4.54	1.36
pentanal	0	-3.03	-4.77	1.74	-0.0273	0.0274	0.28	-4.49	1.46
octanal	0	-2.29	-4.88	2.59	-0.0271	0.0275	0.34	-4.54	2.25
benzaldehyde	0	-4.02	-5.57	1.55	-0.0279	0.0304	0.15	-5.42	1.40
p-hydroxybenzaldehyde	0	-10.48	-10.09	-0.39	-0.0293	0.0823	-1.92	-12.00	1.52
m-hydroxybenzaldehyde	0	-9.51	-9.60	0.09	-0.0278	0.0816	-1.50	-11.09	1.58
acetone	0	-3.85	-5.37	1.52	-0.0285	0.0274	0.01	-5.35	1.50
2-butanone	0	-3.64	-5.00	1.36	-0.0288	0.0269	-0.04	-5.05	1.41
2-pentanone	0	-3.53	-5.03	1.50	-0.0289	0.0268	-0.07	-5.11	1.58
3-pentanone	0	-3.41	-4.64	1.23	-0.0281	0.0247	0.13	-4.51	1.10
2-hexanone	0	-3.29	-5.09	1.80	-0.0288	0.0270	-0.06	-5.15	1.86
2-heptanone	0	-3.04	-5.14	2.10	-0.0290	0.0262	-0.09	-5.23	2.19
4-heptanone	0	-2.93	-4.71	1.78	-0.0282	0.0243	0.11	-4.60	1.67
2-octanone	0	-2.88	-5.19	2.31	-0.0289	0.0261	-0.07	-5.26	2.38
5-nonanone	0	-2.67	-4.80	2.13	-0.0283	0.0240	0.09	-4.71	2.04
3,3-dimethylbutanone	0	-2.89	-4.79	1.90	-0.0289	0.0271	-0.09	-4.88	1.99
cyclopentanone	0	-4.68	-5.38	0.70	-0.0286	0.0256	0.01	-5.37	0.69
acetophenone	0	-4.58	-5.77	1.19	-0.0292	0.0286	-0.17	-5.94	1.36
methyl formate	0	-2.78	-4.98	2.20	-0.0253	0.0363	0.61	-4.37	1.59
ethyl formate	0	-2.65	-4.93	2.28	-0.0258	0.0355	0.54	-4.39	1.74
methyl acetate	0	-3.32	-4.94	1.62	-0.0272	0.0280	0.30	-4.64	1.32
ethyl acetate	0	-3.10	-4.93	1.83	-0.0276	0.0276	0.23	-4.70	1.60

propyl acetate	0	-2.86	-4.95	2.09	-0.0276	0.0275	0.22	-4.73	1.87
butyl acetate	0	-2.55	-5.01	2.46	-0.0276	0.0274	0.23	-4.78	2.23
methyl propanoate	0	-2.93	-4.67	1.74	-0.0267	0.0268	0.42	-4.25	1.32
methyl butanoate	0	-2.83	-4.71	1.88	-0.0268	0.0267	0.39	-4.32	1.49
methyl pentanoate	0	-2.57	-4.78	2.21	-0.0270	0.0264	0.37	-4.41	1.84
methyl hexanoate	0	-2.49	-4.83	2.34	-0.0269	0.0262	0.38	-4.45	1.96
methyl benzoate	0	-3.91	-5.32	1.41	-0.0271	0.0282	0.32	-4.99	1.08
hydrogen	0	2.33	-0.21	2.54	0.0002	0.0212	2.10	1.89	0.44
water	0	-6.31	-7.06	0.75	-0.0269	0.0724	-0.75	-7.81	1.50
water dimer	0	-11.27	-11.59	0.32	-0.0310	0.0804	-2.23	-13.81	2.54
hydrogen peroxide	0	-8.58	-8.11	-0.47	-0.0222	0.0800	-0.39	-8.50	-0.08
methyl peroxide	0	-5.28	-6.01	0.73	-0.0229	0.0782	-0.38	-6.39	1.11
ethyl peroxide	0	-5.32	-5.97	0.65	-0.0233	0.0769	-0.36	-6.33	1.01
1,4-dioxane	0	-5.05	-4.56	-0.49	-0.0259	0.0239	0.59	-3.97	-1.08
methanol	0	-5.11	-4.91	-0.20	-0.0271	0.0685	-0.58	-5.49	0.38
ethanol	0	-5.01	-4.64	-0.37	-0.0270	0.0672	-0.51	-5.14	0.13
1-propanol	0	-4.83	-4.65	-0.18	-0.0270	0.0661	-0.46	-5.11	0.28
isopropanol	0	-4.76	-4.57	-0.19	-0.0278	0.0629	-0.51	-5.07	0.31
1-butanol	0	-4.72	-4.70	-0.02	-0.0271	0.0658	-0.47	-5.18	0.46
t-butanol	0	-4.51	-4.40	-0.11	-0.0275	0.0617	-0.40	-4.80	0.29
1-pentanol	0	-4.47	-4.90	0.43	-0.0277	0.0643	-0.54	-5.44	0.97
1-hexanol	0	-4.36	-4.97	0.61	-0.0278	0.0655	-0.61	-5.57	1.21
1-heptanol	0	-4.24	-5.05	0.81	-0.0278	0.0636	-0.53	-5.58	1.34
1-octanol	0	-4.09	-4.91	0.82	-0.0277	0.0649	-0.56	-5.48	1.39
allyl alcohol	0	-5.08	-4.87	-0.21	-0.0267	0.0670	-0.45	-5.32	0.24
cyclopentanol	0	-5.49	-4.34	-1.15	-0.0278	0.0599	-0.39	-4.73	-0.76
2-methoxyethanol	0	-6.77	-6.49	-0.28	-0.0262	0.0697	-0.47	-6.96	0.19
2,2,2-trifluoroethanol	0	-4.31	-7.59	3.28	-0.0205	0.0791	-0.13	-7.72	3.41
1,1,1-trifluoropropan-2-ol	0	-4.16	-5.33	1.17	-0.0229	0.0721	-0.02	-5.36	1.20
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-5.90	2.13	-0.0176	0.0823	-0.07	-5.97	2.20
phenol	0	-6.62	-6.18	-0.44	-0.0215	0.0769	-0.10	-6.28	-0.34
p-bromophenol	0	-7.13	-6.73	-0.40	-0.0198	0.0783	-0.01	-6.74	-0.39
o-cresol	0	-5.87	-5.76	-0.11	-0.0210	0.0760	0.01	-5.75	-0.12
m-cresol	0	-5.49	-6.13	0.64	-0.0219	0.0773	-0.18	-6.31	0.82
p-cresol	0	-6.14	-6.06	-0.08	-0.0221	0.0769	-0.18	-6.24	0.10

1,2-ethanediol	0	-9.30	-7.89	-1.41	-0.0287	0.0736	-1.22	-9.10	-0.20
acetic acid	0	-6.70	-7.02	0.32	-0.0263	0.0827	-1.26	-8.28	1.58
propanoic acid	0	-6.47	-6.74	0.27	-0.0258	0.0818	-1.11	-7.84	1.37
butanoic acid	0	-6.36	-6.75	0.39	-0.0259	0.0817	-1.11	-7.86	1.50
pentanoic acid	0	-6.16	-6.81	0.65	-0.0259	0.0821	-1.13	-7.95	1.79
hexanoic acid	0	-6.21	-6.86	0.65	-0.0260	0.0811	-1.08	-7.94	1.73
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-11.81	-0.15	-0.0234	0.0830	-0.78	-12.59	0.63
ammonia	0	-4.29	-4.42	0.13	-0.0305	0.0424	-0.64	-5.06	0.77
methylamine	0	-4.56	-3.55	-1.01	-0.0302	0.0400	-0.54	-4.10	-0.46
ethylamine	0	-4.50	-3.63	-0.87	-0.0304	0.0387	-0.57	-4.21	-0.29
butylamine	0	-4.29	-3.73	-0.56	-0.0305	0.0381	-0.59	-4.32	0.03
propylamine	0	-4.39	-3.68	-0.71	-0.0305	0.0388	-0.59	-4.27	-0.12
pentylamine	0	-4.10	-3.77	-0.33	-0.0306	0.0378	-0.62	-4.39	0.29
dimethylamine	0	-4.29	-2.65	-1.64	-0.0289	0.0395	-0.20	-2.85	-1.44
diethylamine	0	-4.07	-2.57	-1.50	-0.0289	0.0370	-0.15	-2.72	-1.35
dipropylamine	0	-3.66	-2.65	-1.01	-0.0287	0.0370	-0.10	-2.75	-0.91
trimethylamine	0	-3.23	-1.70	-1.53	-0.0273	0.0191	0.33	-1.37	-1.86
azetidine	0	-5.56	-2.89	-2.67	-0.0302	0.0379	-0.50	-3.39	-2.17
pyrrolidine	0	-5.48	-3.13	-2.35	-0.0302	0.0379	-0.50	-3.63	-1.85
piperidine	0	-5.11	-2.30	-2.81	-0.0284	0.0386	-0.05	-2.35	-2.76
2-methoxyethanamine	0	-6.55	-5.67	-0.88	-0.0293	0.0406	-0.31	-5.99	-0.56
1,2-ethanediamine	0	-9.72	-6.96	-2.76	-0.0295	0.0405	-0.36	-7.32	-2.40
nitromethane	0	-3.95	-6.70	2.75	-0.0204	0.0390	1.29	-5.41	1.46
nitroethane	0	-3.71	-6.32	2.61	-0.0211	0.0356	1.24	-5.08	1.37
1-nitropropane	0	-3.34	-6.25	2.91	-0.0212	0.0350	1.25	-5.00	1.66
2-nitropropane	0	-3.14	-5.75	2.61	-0.0215	0.0332	1.23	-4.52	1.38
1-nitrobutane	0	-3.08	-6.29	3.21	-0.0212	0.0349	1.24	-5.04	1.96
nitrobenzene	0	-4.12	-5.84	1.72	-0.0210	0.0339	1.27	-4.56	0.44
2-methyl-1-nitrobenzene	0	-3.59	-5.58	1.99	-0.0221	0.0317	1.16	-4.42	0.83
pyridine	0	-4.70	-4.14	-0.56	-0.0302	0.0306	-0.43	-4.57	-0.13
2-methylpyridine	0	-4.63	-3.82	-0.81	-0.0303	0.0292	-0.44	-4.26	-0.37
3-methylpyridine	0	-4.77	-4.22	-0.55	-0.0307	0.0288	-0.57	-4.79	0.02
4-methylpyridine	0	-4.94	-4.35	-0.59	-0.0310	0.0277	-0.64	-4.99	0.05
4-ethylpyridine	0	-4.74	-4.36	-0.38	-0.0311	0.0277	-0.66	-5.02	0.28
2,4-dimethylpyridine	0	-4.86	-4.01	-0.85	-0.0310	0.0264	-0.64	-4.65	-0.21

2,5-dimethylpyridine	0	-4.72	-3.87	-0.85	-0.0307	0.0278	-0.54	-4.41	-0.31
2,6-dimethylpyridine	0	-4.60	-3.51	-1.09	-0.0302	0.0286	-0.42	-3.94	-0.66
3,4-dimethylpyridine	0	-5.22	-4.52	-0.70	-0.0315	0.0270	-0.78	-5.30	0.08
3,5-dimethylpyridine	0	-4.84	-4.29	-0.55	-0.0312	0.0278	-0.71	-5.00	0.16
aniline	0	-5.49	-5.73	0.24	-0.0220	0.0517	0.86	-4.87	-0.62
N-methylaniline	0	-4.68	-4.64	-0.04	-0.0189	0.0510	1.22	-3.41	-1.27
2-methylaniline	0	-5.56	-5.30	-0.26	-0.0224	0.0497	0.85	-4.45	-1.11
3-methylaniline	0	-5.67	-5.63	-0.04	-0.0224	0.0506	0.83	-4.80	-0.87
4-methylaniline	0	-5.55	-5.55	0.00	-0.0227	0.0492	0.82	-4.73	-0.82
N-ethylaniline	0	-4.62	-4.54	-0.08	-0.0168	0.0516	1.38	-3.16	-1.46
3-aminoaniline	0	-9.92	-9.10	-0.82	-0.0227	0.0503	0.81	-8.29	-1.63
N,N-dimethylaniline	0	-3.58	-3.56	-0.02	-0.0148	0.0241	1.85	-1.71	-1.87
piperazine	0	-7.40	-4.30	-3.10	-0.0281	0.0394	0.00	-4.30	-3.10
N-methylpiperazine	0	-7.77	-3.47	-4.30	-0.0279	0.0399	0.04	-3.43	-4.34
N,N'-dimethylpiperazine	0	-7.58	-2.61	-4.97	-0.0262	0.0192	0.55	-2.06	-5.52
1-methylthymine	0	-10.40	-11.96	1.56	-0.0301	0.0696	-1.35	-13.31	2.91
9-methyladenine	0	-13.60	-10.35	-3.25	-0.0304	0.0628	-1.13	-11.48	-2.12
acetamide	0	-9.71	-9.19	-0.52	-0.0316	0.0632	-1.52	-10.70	0.99
E-N-methylacetamide	0	-10.00	-8.34	-1.66	-0.0330	0.0559	-1.71	-10.05	0.05
Z-N-methylacetamide	0	-10.00	-7.87	-2.13	-0.0331	0.0620	-1.93	-9.80	-0.20
benzamide	0	-10.90	-9.21	-1.69	-0.0307	0.0628	-1.24	-10.45	-0.45
2,6-dichlorothiobenzamide	0	-10.81	-10.52	-0.29	-0.0195	0.0737	0.29	-10.23	-0.58
urea	0	-13.80	-11.47	-2.33	-0.0310	0.0612	-1.27	-12.74	-1.06
1,1-dimethyl-3-phenylurea	0	-9.63	-8.85	-0.78	-0.0303	0.0561	-0.89	-9.74	0.11
hydrazine	0	-6.26	-6.22	-0.04	-0.0285	0.0427	-0.15	-6.37	0.11
methylhydrazine	0	-5.31	-5.54	0.23	-0.0284	0.0426	-0.11	-5.65	0.34
1,1-dimethylhydrazine	0	-4.48	-4.35	-0.13	-0.0285	0.0428	-0.15	-4.49	0.01
2-methylpyrazine	0	-5.57	-4.54	-1.03	-0.0269	0.0301	0.35	-4.19	-1.38
2-ethylpyrazine	0	-5.51	-4.21	-1.30	-0.0270	0.0299	0.34	-3.87	-1.64
morpholine	0	-7.17	-4.56	-2.61	-0.0274	0.0416	0.13	-4.43	-2.74
N-methylmorpholine	0	-6.34	-3.61	-2.73	-0.0270	0.0216	0.37	-3.24	-3.10
acetonitrile	0	-3.89	-6.74	2.85	-0.0280	0.0363	0.06	-6.68	2.79
butanonitrile	0	-3.64	-6.14	2.50	-0.0281	0.0331	0.08	-6.06	2.42
propionitrile	0	-3.85	-6.37	2.52	-0.0282	0.0334	0.05	-6.32	2.47
benzonitrile	0	-4.10	-6.33	2.23	-0.0276	0.0339	0.18	-6.15	2.05

2,6-dichlorobenzonitrile	0	-5.22	-6.66	1.44	-0.0266	0.0370	0.36	-6.30	1.08
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-8.30	-0.70	-0.0265	0.0696	-0.52	-8.82	-0.18
trimethylphosphate	0	-8.70	-8.34	-0.36	-0.0299	0.0299	-0.36	-8.70	0.00
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-7.65	1.04	-0.0264	0.0418	0.33	-7.32	0.71
phosphine	0	0.60	-0.66	1.26	-0.0092	0.0228	2.05	1.38	-0.78
hydrogen sulfide	0	-0.70	-2.31	1.61	-0.0110	0.0384	1.89	-0.43	-0.27
dimethyl sulfide	0	-1.54	-2.58	1.04	-0.0166	0.0257	1.74	-0.84	-0.70
diethyl sulfide	0	-1.43	-2.45	1.02	-0.0173	0.0212	1.70	-0.74	-0.69
dipropyl sulfide	0	-1.27	-2.57	1.30	-0.0176	0.0208	1.69	-0.89	-0.38
bis(2-chloroethyl)sulfide	0	-3.92	-5.34	1.42	-0.0121	0.0311	1.93	-3.42	-0.50
dimethyl disulfide	0	-1.83	-2.98	1.15	-0.0122	0.0281	1.94	-1.04	-0.79
diethyl disulfide	0	-1.63	-2.69	1.06	-0.0127	0.0257	1.94	-0.75	-0.88
methanethiol	0	-1.24	-2.47	1.23	-0.0143	0.0331	1.82	-0.65	-0.59
ethanethiol	0	-1.30	-2.47	1.17	-0.0145	0.0320	1.82	-0.65	-0.65
1-propanethiol	0	-1.05	-2.53	1.48	-0.0147	0.0316	1.81	-0.72	-0.33
thiophene	0	-1.42	-2.62	1.20	-0.0063	0.0330	2.02	-0.60	-0.82
thiophenol	0	-2.55	-3.60	1.05	-0.0099	0.0373	1.93	-1.67	-0.88
thioanisole	0	-2.73	-3.75	1.02	-0.0124	0.0290	1.93	-1.82	-0.91
tetramethylsilane	0	3.04	-0.97	4.01	-0.0028	0.0184	2.11	1.14	1.90
acetylene	-1	-76.50	-66.12	-10.38	-0.0530	0.0162	-13.81	-79.93	3.43
acetonitrile	-1	-66.60	-60.09	-6.51	-0.0509	0.0011	-11.83	-71.92	5.32
cyanamide	-1	-72.20	-63.73	-8.47	-0.0514	0.0197	-12.26	-75.99	3.79
aniline	-1	-62.90	-54.41	-8.49	-0.0521	0.0085	-12.90	-67.31	4.41
diphenylamine	-1	-54.60	-47.04	-7.56	-0.0451	0.0123	-7.25	-54.29	-0.31
hydrogen cyanide	-1	-70.20	-65.98	-4.22	-0.0502	-0.0354	-11.16	-77.14	6.94
formic acid	-1	-76.20	-64.80	-11.40	-0.0505	-0.0063	-11.44	-76.25	0.05
acetic acid	-1	-77.60	-63.80	-13.80	-0.0518	0.0068	-12.62	-76.42	-1.18
propanoic acid	-1	-76.20	-61.79	-14.41	-0.0518	0.0074	-12.66	-74.45	-1.75
hexanoic acid	-1	-74.60	-60.86	-13.74	-0.0518	0.0143	-12.65	-73.51	-1.09
acrylic acid	-1	-74.00	-62.43	-11.57	-0.0515	0.0154	-12.33	-74.76	0.76
pyruvic acid	-1	-68.50	-61.35	-7.15	-0.0490	0.0175	-10.17	-71.51	3.01
benzoic acid	-1	-71.20	-59.46	-11.74	-0.0509	0.0190	-11.81	-71.27	0.07
methanol	-1	-95.00	-66.52	-28.48	-0.0611	-0.0161	-23.34	-89.86	-5.14
ethanol	-1	-90.70	-62.84	-27.86	-0.0610	0.0010	-23.24	-86.08	-4.62
1-propanol	-1	-88.30	-62.30	-26.00	-0.0612	0.0074	-23.54	-85.84	-2.46

isopropanol	-1	-86.30	-60.17	-26.13	-0.0606	0.0014	-22.65	-82.81	-3.49
2-butanol	-1	-84.20	-57.42	-26.78	-0.0598	0.0021	-21.61	-79.03	-5.17
t-butanol	-1	-82.30	-58.17	-24.13	-0.0601	0.0022	-22.05	-80.22	-2.08
allyl alcohol	-1	-86.60	-62.05	-24.55	-0.0602	0.0091	-22.15	-84.21	-2.39
benzyl alcohol	-1	-85.10	-57.90	-27.20	-0.0593	0.0152	-20.97	-78.87	-6.23
2-methoxyethanol	-1	-89.40	-63.50	-25.90	-0.0608	0.0135	-22.98	-86.48	-2.92
phenol	-1	-71.90	-56.35	-15.55	-0.0534	0.0094	-14.25	-70.60	-1.30
2-methylphenol	-1	-70.20	-54.52	-15.68	-0.0534	0.0083	-14.22	-68.74	-1.46
3-methylphenol	-1	-71.10	-56.04	-15.06	-0.0537	0.0120	-14.53	-70.58	-0.52
4-methylphenol	-1	-72.00	-56.01	-15.99	-0.0541	0.0109	-14.89	-70.90	-1.10
1,2-ethanediol	-1	-85.30	-66.57	-18.73	-0.0610	0.0556	-23.72	-90.29	4.99
3-hydroxyphenol	-1	-73.80	-58.07	-15.73	-0.0527	0.0620	-14.19	-72.27	-1.53
4-hydroxyphenol	-1	-77.60	-59.51	-18.09	-0.0542	0.0599	-15.69	-75.20	-2.40
methyl hydroperoxide	-1	-93.20	-68.70	-24.50	-0.0606	0.0036	-22.65	-91.35	-1.85
ethyl hydroperoxide	-1	-89.20	-67.99	-21.21	-0.0608	0.0108	-22.99	-90.98	1.78
acetaldehyde	-1	-76.50	-61.54	-14.96	-0.0547	-0.0007	-15.60	-77.14	0.64
acetone	-1	-76.20	-60.02	-16.18	-0.0551	0.0042	-16.01	-76.03	-0.17
3-pentanone	-1	-73.70	-55.08	-18.62	-0.0541	0.0067	-14.91	-69.99	-3.71
water	-1	-104.70	-77.45	-27.25	-0.0650	-0.0010	-29.09	-106.54	1.84
hydrogen peroxide	-1	-97.30	-75.11	-22.19	-0.0612	0.0372	-23.64	-98.74	1.44
hydroperoxyl radical	-1	-83.30	-71.82	-11.48	-0.0537	-0.0426	-14.50	-86.32	3.02
2-nitrophenol	-1	-60.10	-54.08	-6.02	-0.0472	0.0174	-8.73	-62.81	2.71
3-nitrophenol	-1	-61.90	-51.06	-10.84	-0.0497	0.0217	-10.80	-61.85	-0.05
4-nitrophenol	-1	-57.80	-49.57	-8.23	-0.0454	0.0186	-7.44	-57.01	-0.79
nitromethane	-1	-76.50	-62.38	-14.12	-0.0495	0.0100	-10.62	-73.00	-3.50
4-nitroaniline	-1	-57.40	-49.41	-7.99	-0.0438	0.0189	-6.37	-55.79	-1.61
acetamide	-1	-80.20	-61.50	-18.70	-0.0522	0.0053	-13.03	-74.53	-5.67
methanethiol	-1	-73.80	-61.18	-12.62	-0.0428	0.0018	-5.73	-66.91	-6.89
ethanethiol	-1	-71.80	-58.70	-13.10	-0.0427	0.0055	-5.66	-64.37	-7.43
1-propanethiol	-1	-70.50	-58.48	-12.02	-0.0428	0.0107	-5.76	-64.23	-6.27
thiophenol	-1	-63.40	-53.78	-9.62	-0.0386	0.0148	-3.49	-57.27	-6.13
hydrogen sulfide	-1	-72.10	-62.87	-9.23	-0.0416	-0.0034	-5.04	-67.91	-4.19
dimethyl sulfoxide	-1	-67.70	-57.70	-10.00	-0.0516	0.0106	-12.43	-70.13	2.43
hydrofluoric acid	-1	-104.40	-83.59	-20.81	-0.0691	-0.0691	-36.07	-119.66	15.26
hydrochloric acid	-1	-74.50	-67.08	-7.42	-0.0428	-0.0428	-5.73	-72.81	-1.69

hydrobromic acid	-1	-68.30	-62.92	-5.38	-0.0371	-0.0371	-2.77	-65.69	-2.61
chloroform	-1	-54.10	-50.52	-3.58	-0.0361	-0.0068	-2.36	-52.87	-1.23
trifluoroacetic acid	-1	-59.30	-57.24	-2.06	-0.0459	0.0244	-7.83	-65.07	5.77
chloroacetic acid	-1	-69.70	-58.83	-10.87	-0.0480	0.0166	-9.35	-68.18	-1.52
dichloroacetic acid	-1	-62.30	-55.46	-6.84	-0.0455	0.0232	-7.52	-62.98	0.68
2,2,2-trifluoroethanol	-1	-77.50	-59.64	-17.86	-0.0576	0.0078	-18.82	-78.46	0.96
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-54.87	-10.63	-0.0537	0.0141	-14.56	-69.43	3.93
2-chlorophenol	-1	-66.10	-53.84	-12.26	-0.0513	0.0146	-12.20	-66.04	-0.06
4-chlorophenol	-1	-66.00	-52.41	-13.59	-0.0518	0.0146	-12.60	-65.01	-0.99
methylamine	1	-76.40	-75.10	-1.30	0.0267	0.1051	-1.86	-76.97	0.57
n-propylamine	1	-71.50	-69.72	-1.78	0.0066	0.1034	-1.65	-71.37	-0.13
isopropylamine	1	-69.60	-67.89	-1.71	0.0093	0.1009	-1.36	-69.25	-0.35
tert-butylamine	1	-67.30	-65.06	-2.24	0.0092	0.0988	-1.13	-66.19	-1.11
cyclohexanamine	1	-68.70	-64.74	-3.96	0.0064	0.0995	-1.20	-65.95	-2.75
allylamine	1	-72.00	-70.09	-1.91	-0.0051	0.1051	-1.87	-71.96	-0.04
dimethylamine	1	-68.60	-67.24	-1.36	0.0244	0.0998	-1.24	-68.48	-0.12
diethylamine	1	-63.40	-60.82	-2.58	0.0105	0.0929	-0.52	-61.34	-2.06
di-n-propylamine	1	-60.50	-58.46	-2.04	0.0069	0.0928	-0.51	-58.97	-1.53
diallylamine	1	-61.60	-59.33	-2.27	-0.0039	0.0948	-0.72	-60.04	-1.56
trimethylamine	1	-61.10	-60.59	-0.51	0.0236	0.0958	-0.81	-61.39	0.29
triethylamine	1	-54.60	-52.72	-1.88	0.0082	0.0819	0.37	-52.35	-2.25
aniline	1	-72.40	-68.92	-3.48	0.0033	0.1076	-2.18	-71.11	-1.29
2-methylaniline	1	-70.30	-66.50	-3.80	0.0022	0.1045	-1.79	-68.29	-2.01
3-methylaniline	1	-69.60	-67.20	-2.40	0.0020	0.1064	-2.02	-69.22	-0.38
4-methylaniline	1	-69.80	-67.02	-2.78	0.0030	0.1060	-1.97	-68.99	-0.81
3-aminoaniline	1	-65.80	-68.80	3.00	-0.0112	0.1054	-1.99	-70.79	4.99
N-methylaniline	1	-62.60	-61.41	-1.19	0.0028	0.0998	-1.24	-62.64	0.04
N-ethylaniline	1	-62.20	-58.48	-3.72	0.0027	0.0968	-0.91	-59.39	-2.81
N,N-dimethylaniline	1	-57.20	-55.18	-2.02	0.0028	0.0930	-0.54	-55.72	-1.48
4-methyl-N,N-dimethylaniline	1	-55.90	-53.66	-2.24	0.0026	0.0917	-0.42	-54.08	-1.82
N,N-diethylaniline	1	-54.00	-50.75	-3.25	0.0023	0.0850	0.15	-50.60	-3.40
1-aminonaphthalene	1	-67.40	-65.20	-2.20	0.0010	0.1082	-2.26	-67.45	0.05
aziridine	1	-70.90	-69.04	-1.86	0.0263	0.1054	-1.89	-70.94	0.04
azetidine	1	-67.70	-65.26	-2.44	0.0164	0.0983	-1.07	-66.32	-1.38
pyrrolidine	1	-66.00	-62.81	-3.19	0.0107	0.0968	-0.91	-63.72	-2.28

piperidine	1	-64.20	-60.89	-3.31	0.0124	0.0975	-0.99	-61.88	-2.32
azacycloheptane	1	-63.30	-59.20	-4.10	0.0075	0.0975	-0.98	-60.18	-3.12
pyrrole	1	-61.40	-61.03	-0.37	0.0147	0.1026	-1.56	-62.59	1.19
pyridine	1	-61.10	-59.23	-1.87	0.0176	0.1040	-1.72	-60.95	-0.15
quinoline	1	-56.00	-53.19	-2.81	0.0068	0.0967	-0.90	-54.09	-1.91
piperazine	1	-66.00	-62.95	-3.05	-0.0167	0.0980	-1.39	-64.34	-1.66
acetonitrile	1	-75.30	-69.42	-5.88	0.0335	0.1522	-11.39	-80.81	5.51
ammonia	1	-85.20	-84.89	-0.31	0.0613	0.1123	-2.84	-87.73	2.53
hydrazine	1	-84.60	-82.34	-2.26	-0.0053	0.1107	-2.61	-84.96	0.36
methanol	1	-93.00	-81.49	-11.51	0.0173	0.1537	-11.84	-93.33	0.33
ethanol	1	-88.40	-75.62	-12.78	0.0095	0.1496	-10.64	-86.26	-2.14
dimethyl ether	1	-79.70	-68.86	-10.84	0.0140	0.1445	-9.25	-78.11	-1.59
diethyl ether	1	-71.50	-60.46	-11.04	0.0094	0.1287	-5.64	-66.10	-5.40
acetone	1	-77.10	-65.60	-11.50	0.0080	0.1297	-5.85	-71.44	-5.66
acetophenone	1	-64.50	-54.20	-10.30	0.0038	0.1084	-2.29	-56.49	-8.01
water	1	-110.30	-98.43	-11.87	0.0222	0.1686	-16.81	-115.24	4.94
4-methoxyaniline	1	-71.20	-67.32	-3.88	-0.0158	0.1062	-2.29	-69.62	-1.58
4-nitroaniline	1	-75.90	-80.47	4.57	-0.0149	0.1126	-3.13	-83.60	7.70
morpholine	1	-69.60	-66.79	-2.81	-0.0140	0.1009	-1.55	-68.34	-1.26
acetamide	1	-73.90	-70.66	-3.24	0.0026	0.1235	-4.66	-75.32	1.42
benzamide	1	-67.20	-62.38	-4.82	0.0014	0.1196	-3.97	-66.35	-0.85
dimethyl sulfide	1	-64.50	-61.85	-2.65	0.0227	0.0763	0.74	-61.11	-3.39
dimethyl sulfoxide	1	-67.70	-62.85	-4.85	-0.0005	0.1198	-4.01	-66.86	-0.84
3-chloroaniline	1	-74.70	-71.44	-3.26	-0.0038	0.1094	-2.43	-73.87	-0.83
4-chloroaniline	1	-74.10	-71.60	-2.50	-0.0018	0.1099	-2.49	-74.09	-0.01
PEARSON			0.99					1.00	

Table S 6-3

Electric field extrema (a. u.), hydration free energies (kcal/mol) and related errors from the B3LYP/G3large method for the cavity surface with constant density = 0.002 a. u.

Molecule	Chrg	ΔG_{Exp}	$\Delta G_{\text{SS(V)PE}}$	$\Delta G_{\text{Exp}} - \Delta G_{\text{SS(V)PE}}$	F_{min}	F_{max}	ΔG_{FESR}	$\Delta G_{\text{SS(V)PE}} + \Delta G_{\text{FESR}}$	ΔG_{Err}
methane	0	2.00	-0.50	2.50	0.0033	0.0337	3.73	3.23	-1.23
ethane	0	1.83	-0.51	2.34	0.0029	0.0302	3.73	3.22	-1.39
n-propane	0	1.96	-0.62	2.58	0.0027	0.0298	3.73	3.11	-1.15
n-butane	0	2.08	-0.72	2.80	0.0027	0.0299	3.73	3.01	-0.93
n-pentane	0	2.33	-0.82	3.15	0.0024	0.0296	3.73	2.91	-0.58
n-hexane	0	2.49	-0.91	3.40	0.0026	0.0298	3.73	2.82	-0.33
n-heptane	0	2.62	-1.00	3.62	0.0025	0.0289	3.73	2.74	-0.12
n-octane	0	2.89	-1.08	3.97	0.0025	0.0287	3.73	2.65	0.24
2-methylpropane	0	2.32	-0.79	3.11	0.0027	0.0298	3.73	2.94	-0.62
2,2-dimethylpropane	0	2.50	-1.00	3.50	0.0028	0.0298	3.73	2.74	-0.24
2-methylpentane	0	2.52	-0.96	3.48	0.0020	0.0297	3.73	2.78	-0.26
2,4-dimethylpentane	0	2.88	-1.14	4.02	0.0025	0.0301	3.73	2.59	0.29
2,2,4-trimethylpentane	0	2.85	-1.31	4.16	0.0013	0.0300	3.73	2.42	0.43
cyclopropane	0	0.75	-1.62	2.37	-0.0069	0.0359	3.73	2.11	-1.36
cyclopentane	0	1.20	-0.69	1.89	0.0021	0.0290	3.73	3.04	-1.84
cyclohexane	0	1.23	-0.66	1.89	0.0026	0.0275	3.73	3.08	-1.85
methylcyclohexane	0	1.71	-0.82	2.53	0.0023	0.0293	3.73	2.92	-1.21
cis-1,2-dimethylcyclohexane	0	1.58	-0.96	2.54	0.0012	0.0296	3.73	2.77	-1.19
ethene	0	1.27	-1.75	3.02	-0.0091	0.0409	3.72	1.96	-0.69
propene	0	1.27	-1.81	3.08	-0.0106	0.0381	3.71	1.90	-0.63
1-butene	0	1.38	-1.84	3.22	-0.0110	0.0374	3.70	1.86	-0.48
1-pentene	0	1.66	-1.95	3.61	-0.0110	0.0370	3.70	1.75	-0.09
E-2-pentene	0	1.34	-1.73	3.07	-0.0112	0.0351	3.70	1.97	-0.63
1-hexene	0	1.68	-2.10	3.78	-0.0105	0.0376	3.71	1.61	0.07
2-methylpropene	0	1.16	-1.93	3.09	-0.0115	0.0358	3.70	1.77	-0.61
s-trans-1,3-butadiene	0	0.61	-2.79	3.40	-0.0067	0.0416	3.73	0.94	-0.33
cyclopentene	0	0.56	-1.58	2.14	-0.0116	0.0390	3.70	2.12	-1.56
ethyne	0	-0.01	-5.04	5.03	-0.0100	0.0800	3.69	-1.35	1.34
propyne	0	-0.31	-4.43	4.12	-0.0134	0.0732	3.66	-0.78	0.47
1-butyne	0	-0.16	-4.33	4.17	-0.0137	0.0732	3.65	-0.68	0.52
1-pentyne	0	0.01	-4.23	4.24	-0.0144	0.0726	3.64	-0.59	0.60
1-hexyne	0	0.29	-4.55	4.84	-0.0136	0.0721	3.65	-0.90	1.19

butenyne	0	0.04	-4.61	4.65	-0.0121	0.0762	3.67	-0.94	0.98
benzene	0	-0.87	-3.24	2.37	-0.0003	0.0417	3.73	0.49	-1.36
ethylbenzene	0	-0.80	-3.33	2.53	-0.0017	0.0406	3.73	0.40	-1.20
naphthalene	0	-2.39	-4.49	2.10	-0.0016	0.0420	3.73	-0.76	-1.63
anthracene	0	-4.23	-5.70	1.47	-0.0016	0.0422	3.73	-1.97	-2.26
toluene	0	-0.89	-3.27	2.38	-0.0016	0.0407	3.73	0.46	-1.35
p-xylene	0	-0.81	-3.23	2.42	-0.0031	0.0384	3.73	0.50	-1.31
m-xylene	0	-0.84	-3.28	2.44	-0.0031	0.0399	3.73	0.46	-1.30
o-xylene	0	-0.90	-3.39	2.49	-0.0030	0.0395	3.73	0.35	-1.25
fluoromethane	0	-0.22	-3.58	3.36	-0.0189	0.0429	3.53	-0.05	-0.17
chloromethane	0	-0.56	-3.39	2.83	-0.0069	0.0486	3.72	0.33	-0.89
bromomethane	0	-0.82	-3.26	2.44	-0.0039	0.0495	3.73	0.47	-1.29
chlorofluoromethane	0	-0.77	-4.94	4.17	-0.0102	0.0593	3.70	-1.24	0.47
dichloromethane	0	-1.36	-4.62	3.26	-0.0014	0.0619	3.72	-0.90	-0.46
dibromomethane	0	-2.11	-4.59	2.48	0.0008	0.0620	3.72	-0.86	-1.25
chlorodifluoromethane	0	-0.50	-4.51	4.01	-0.0034	0.0721	3.71	-0.80	0.30
chloroform	0	-1.07	-4.10	3.03	0.0033	0.0730	3.71	-0.39	-0.68
chloroethane	0	-0.63	-3.46	2.83	-0.0082	0.0460	3.72	0.26	-0.89
bromoethane	0	-0.70	-3.34	2.64	-0.0051	0.0469	3.73	0.38	-1.08
bromoform	0	-1.98	-4.50	2.52	0.0046	0.0721	3.71	-0.78	-1.20
tetrafluoromethane	0	3.16	-1.59	4.75	0.0029	0.0643	3.72	2.13	1.03
difluorodichloromethane	0	1.69	-1.72	3.41	0.0022	0.0500	3.73	2.01	-0.32
fluorotrichloromethane	0	0.82	-1.91	2.73	0.0016	0.0486	3.73	1.82	-1.00
bromotrifluoromethane	0	1.79	-1.93	3.72	0.0024	0.0634	3.72	1.79	0.00
bromotrichloromethane	0	-0.93	-2.46	1.53	0.0062	0.0572	3.73	1.26	-2.19
hexafluoroethane	0	3.94	-1.91	5.85	0.0028	0.0648	3.72	1.81	2.13
hexachloroethane	0	-1.40	-2.93	1.53	0.0032	0.0466	3.73	0.80	-2.20
chloropentafluoroethane	0	2.86	-1.93	4.79	0.0019	0.0617	3.72	1.79	1.07
1,1,2-trichloro-1,2,2-trifluoroethane	0	1.77	-2.24	4.01	-0.0001	0.0492	3.73	1.49	0.28
1-bromo-1,2,2,2-tetrafluoroethane	0	0.52	-5.17	5.69	-0.0050	0.0739	3.71	-1.46	1.98
1-bromo-1-chloro-2,2,2-trifluoroethane	0	-0.13	-4.91	4.78	-0.0016	0.0742	3.71	-1.20	1.07
1-chloro-2,2,2-trifluoroethane	0	0.06	-5.40	5.46	-0.0035	0.0631	3.72	-1.68	1.74
1,1,1,2-tetrachloroethane	0	-1.15	-4.88	3.73	-0.0014	0.0614	3.72	-1.16	0.01
1,1,1-trichloroethane	0	-0.25	-3.39	3.14	0.0003	0.0484	3.73	0.34	-0.59
1,1,2-trichloroethane	0	-1.95	-5.85	3.90	-0.0040	0.0645	3.72	-2.13	0.18

1,1-difluoroethane	0	-0.11	-4.90	4.79	-0.0134	0.0526	3.67	-1.23	1.12
1-bromo-2-chloroethane	0	-1.95	-4.96	3.01	-0.0050	0.0525	3.73	-1.23	-0.72
octafluoropropane	0	4.28	-2.25	6.53	0.0028	0.0634	3.72	1.47	2.81
2-chloropropane	0	-0.25	-3.53	3.28	-0.0092	0.0444	3.72	0.19	-0.44
1-chloropropane	0	-0.27	-3.50	3.23	-0.0083	0.0452	3.72	0.22	-0.49
1-bromopropane	0	-0.56	-3.41	2.85	-0.0053	0.0461	3.73	0.32	-0.88
2-bromopropane	0	-0.48	-3.42	2.94	-0.0061	0.0455	3.73	0.31	-0.79
2-chlorobutane	0	0.07	-3.40	3.47	-0.0092	0.0434	3.72	0.32	-0.25
1-bromobutane	0	-0.41	-3.49	3.08	-0.0053	0.0459	3.73	0.24	-0.65
1-chloropentane	0	0.07	-3.72	3.79	-0.0083	0.0450	3.72	0.00	0.07
2-chloropentane	0	0.07	-3.46	3.53	-0.0093	0.0433	3.72	0.25	-0.18
1-bromopentane	0	-0.08	-3.61	3.53	-0.0055	0.0460	3.73	0.12	-0.20
1-bromo-isobutane	0	-0.03	-3.33	3.30	-0.0053	0.0461	3.73	0.39	-0.42
tetrachloroethene	0	0.05	-2.24	2.29	0.0026	0.0456	3.73	1.49	-1.44
trichloroethene	0	-0.39	-3.00	2.61	0.0015	0.0655	3.72	0.72	-1.11
chloroethene	0	-0.59	-2.97	2.38	-0.0041	0.0553	3.73	0.75	-1.34
E-1,2-dichloroethene	0	-0.76	-3.35	2.59	-0.0015	0.0611	3.72	0.37	-1.13
Z-1,2-dichloroethene	0	-1.17	-4.04	2.87	-0.0005	0.0622	3.72	-0.32	-0.85
3-chloropropene	0	-0.57	-4.22	3.65	-0.0072	0.0501	3.72	-0.50	-0.07
3-bromopropene	0	-0.86	-4.34	3.48	-0.0049	0.0507	3.73	-0.62	-0.24
fluorobenzene	0	-0.78	-3.95	3.17	-0.0133	0.0484	3.67	-0.28	-0.50
chlorobenzene	0	-1.12	-3.67	2.55	-0.0043	0.0477	3.73	0.06	-1.18
bromobenzene	0	-1.46	-3.75	2.29	-0.0019	0.0480	3.73	-0.02	-1.44
1,4-dichlorobenzene	0	-1.01	-3.99	2.98	-0.0028	0.0514	3.73	-0.27	-0.74
1,2-dichlorobenzene	0	-1.36	-4.04	2.68	-0.0035	0.0510	3.73	-0.31	-1.05
p-dibromobenzene	0	-2.30	-4.18	1.88	-0.0004	0.0510	3.73	-0.45	-1.85
chlorotoluene	0	-1.92	-5.90	3.98	-0.0080	0.0484	3.72	-2.18	0.26
o-chlorotoluene	0	-1.15	-3.51	2.36	-0.0051	0.0470	3.73	0.22	-1.37
bromotoluene	0	-2.37	-5.79	3.42	-0.0051	0.0502	3.73	-2.06	-0.31
p-bromotoluene	0	-1.39	-3.82	2.43	-0.0024	0.0472	3.73	-0.09	-1.30
2,3-dichlorobiphenyl	0	-2.45	-5.81	3.36	-0.0039	0.0500	3.73	-2.08	-0.37
2,2'-dichlorobiphenyl	0	-2.73	-6.20	3.47	-0.0052	0.0472	3.73	-2.47	-0.26
2,2',3'-trichlorobiphenyl	0	-1.99	-6.24	4.25	-0.0054	0.0504	3.73	-2.51	0.52
1,2-dimethoxyethane	0	-4.84	-5.80	0.96	-0.0293	0.0372	2.77	-3.03	-1.81
anisole	0	-2.45	-5.38	2.93	-0.0250	0.0442	3.18	-2.19	-0.26

dimethyl ether	0	-1.92	-3.72	1.80	-0.0305	0.0373	2.62	-1.10	-0.82
diethyl ether	0	-1.76	-4.00	2.24	-0.0319	0.0343	2.43	-1.57	-0.19
isopropyl ether	0	-0.53	-4.03	3.50	-0.0323	0.0343	2.36	-1.68	1.15
methyl propyl ether	0	-1.66	-3.68	2.02	-0.0306	0.0366	2.61	-1.06	-0.60
methyl isopropyl ether	0	-2.01	-3.76	1.75	-0.0311	0.0360	2.53	-1.23	-0.78
t-butyl methyl ether	0	-2.21	-3.86	1.65	-0.0315	0.0354	2.48	-1.37	-0.84
ethyl phenyl ether	0	-2.22	-5.29	3.07	-0.0252	0.0439	3.17	-2.12	-0.10
tetrahydrofuran	0	-3.47	-4.18	0.71	-0.0326	0.0362	2.32	-1.86	-1.61
tetrahydropyran	0	-3.12	-3.91	0.79	-0.0321	0.0342	2.39	-1.52	-1.60
2,2,2-trifluoroethyl vinyl ether	0	-0.12	-6.49	6.37	-0.0172	0.0549	3.58	-2.91	2.79
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	0	0.11	-7.84	7.95	-0.0100	0.0741	3.69	-4.14	4.25
acetaldehyde	0	-3.50	-6.85	3.35	-0.0310	0.0496	2.55	-4.30	0.80
propanal	0	-3.44	-6.51	3.07	-0.0313	0.0475	2.51	-4.00	0.56
butanal	0	-3.18	-6.76	3.58	-0.0312	0.0479	2.53	-4.24	1.06
pentanal	0	-3.03	-6.68	3.65	-0.0317	0.0462	2.46	-4.23	1.20
octanal	0	-2.29	-6.67	4.38	-0.0311	0.0433	2.54	-4.13	1.84
benzaldehyde	0	-4.02	-7.75	3.73	-0.0321	0.0488	2.39	-5.36	1.34
p-hydroxybenzaldehyde	0	-10.48	-14.26	3.78	-0.0337	0.1258	1.99	-12.27	1.79
m-hydroxybenzaldehyde	0	-9.51	-13.70	4.19	-0.0319	0.1248	2.29	-11.41	1.90
acetone	0	-3.85	-7.33	3.48	-0.0332	0.0449	2.22	-5.12	1.27
2-butanone	0	-3.64	-6.96	3.32	-0.0337	0.0444	2.14	-4.82	1.18
2-pentanone	0	-3.53	-7.03	3.50	-0.0336	0.0440	2.16	-4.87	1.34
3-pentanone	0	-3.41	-6.59	3.18	-0.0323	0.0425	2.37	-4.22	0.81
2-hexanone	0	-3.29	-7.13	3.84	-0.0336	0.0436	2.15	-4.98	1.69
2-heptanone	0	-3.04	-7.21	4.17	-0.0335	0.0433	2.16	-5.05	2.01
4-heptanone	0	-2.93	-6.73	3.80	-0.0325	0.0425	2.33	-4.41	1.48
2-octanone	0	-2.88	-7.19	4.31	-0.0334	0.0434	2.19	-5.00	2.12
5-nonanone	0	-2.67	-6.86	4.19	-0.0325	0.0419	2.33	-4.53	1.86
3,3-dimethylbutanone	0	-2.89	-6.80	3.91	-0.0338	0.0447	2.13	-4.68	1.79
cyclopentanone	0	-4.68	-7.34	2.66	-0.0330	0.0434	2.26	-5.08	0.40
acetophenone	0	-4.58	-8.05	3.47	-0.0339	0.0464	2.11	-5.94	1.36
methyl formate	0	-2.78	-7.19	4.41	-0.0286	0.0581	2.85	-4.34	1.56
ethyl formate	0	-2.65	-7.15	4.50	-0.0292	0.0571	2.78	-4.37	1.72
methyl acetate	0	-3.32	-7.16	3.84	-0.0311	0.0471	2.53	-4.63	1.31
ethyl acetate	0	-3.10	-7.18	4.08	-0.0316	0.0458	2.47	-4.71	1.61

propyl acetate	0	-2.86	-7.22	4.36	-0.0317	0.0463	2.45	-4.77	1.91
butyl acetate	0	-2.55	-7.29	4.74	-0.0315	0.0449	2.47	-4.81	2.26
methyl propanoate	0	-2.93	-6.89	3.96	-0.0308	0.0463	2.58	-4.31	1.38
methyl butanoate	0	-2.83	-6.96	4.13	-0.0310	0.0457	2.55	-4.41	1.58
methyl pentanoate	0	-2.57	-7.05	4.48	-0.0308	0.0456	2.57	-4.47	1.90
methyl hexanoate	0	-2.49	-7.12	4.63	-0.0310	0.0455	2.54	-4.58	2.09
methyl benzoate	0	-3.91	-7.59	3.68	-0.0316	0.0464	2.46	-5.12	1.21
hydrogen	0	2.33	-0.40	2.73	0.0040	0.0375	3.73	3.33	-1.00
water	0	-6.31	-10.15	3.84	-0.0312	0.1126	2.44	-7.72	1.41
water dimer	0	-11.27	-16.42	5.15	-0.0357	0.1210	1.65	-14.77	3.50
hydrogen peroxide	0	-8.58	-11.92	3.34	-0.0251	0.1239	3.05	-8.88	0.30
methyl peroxide	0	-5.28	-8.71	3.43	-0.0258	0.1215	3.00	-5.72	0.44
ethyl peroxide	0	-5.32	-8.71	3.39	-0.0263	0.1186	2.97	-5.75	0.43
1,4-dioxane	0	-5.05	-6.70	1.65	-0.0299	0.0401	2.69	-4.01	-1.04
methanol	0	-5.11	-7.07	1.96	-0.0313	0.1076	2.43	-4.64	-0.47
ethanol	0	-5.01	-6.84	1.83	-0.0314	0.1055	2.43	-4.41	-0.60
1-propanol	0	-4.83	-6.89	2.06	-0.0313	0.1048	2.43	-4.45	-0.38
isopropanol	0	-4.76	-6.85	2.09	-0.0322	0.1009	2.32	-4.53	-0.23
1-butanol	0	-4.72	-6.99	2.27	-0.0314	0.1045	2.43	-4.57	-0.15
t-butanol	0	-4.51	-6.74	2.23	-0.0320	0.0986	2.36	-4.38	-0.13
1-pentanol	0	-4.47	-7.18	2.71	-0.0319	0.1020	2.36	-4.82	0.35
1-hexanol	0	-4.36	-7.17	2.81	-0.0321	0.1035	2.33	-4.84	0.48
1-heptanol	0	-4.24	-7.12	2.88	-0.0321	0.1019	2.33	-4.79	0.55
1-octanol	0	-4.09	-7.27	3.18	-0.0319	0.1005	2.36	-4.91	0.82
allyl alcohol	0	-5.08	-7.40	2.32	-0.0308	0.1059	2.51	-4.89	-0.19
cyclopentanol	0	-5.49	-6.54	1.05	-0.0322	0.0965	2.33	-4.21	-1.28
2-methoxyethanol	0	-6.77	-9.59	2.82	-0.0302	0.1092	2.58	-7.01	0.24
2,2,2-trifluoroethanol	0	-4.31	-10.62	6.31	-0.0235	0.1200	3.18	-7.44	3.13
1,1,1-trifluoropropan-2-ol	0	-4.16	-8.12	3.96	-0.0263	0.1133	2.98	-5.13	0.97
1,1,1,3,3,3-hexafluoropropan-2-ol	0	-3.77	-9.31	5.54	-0.0197	0.1264	3.36	-5.95	2.18
phenol	0	-6.62	-9.07	2.45	-0.0241	0.1186	3.14	-5.93	-0.69
p-bromophenol	0	-7.13	-9.84	2.71	-0.0220	0.1203	3.27	-6.57	-0.56
o-cresol	0	-5.87	-8.63	2.76	-0.0243	0.1178	3.13	-5.50	-0.37
m-cresol	0	-5.49	-9.04	3.55	-0.0246	0.1206	3.10	-5.94	0.45
p-cresol	0	-6.14	-8.97	2.83	-0.0246	0.1203	3.10	-5.87	-0.27

1,2-ethanediol	0	-9.30	-11.34	2.04	-0.0331	0.1141	2.14	-9.20	-0.10
acetic acid	0	-6.70	-10.43	3.73	-0.0301	0.1291	2.52	-7.91	1.21
propanoic acid	0	-6.47	-10.15	3.68	-0.0293	0.1277	2.62	-7.53	1.06
butanoic acid	0	-6.36	-10.20	3.84	-0.0294	0.1277	2.61	-7.59	1.23
pentanoic acid	0	-6.16	-10.31	4.15	-0.0294	0.1286	2.61	-7.71	1.55
hexanoic acid	0	-6.21	-10.38	4.17	-0.0295	0.1258	2.61	-7.77	1.56
4-amino-3,5,6-trichloropyridine-2-carboxylic acid	0	-11.96	-17.62	5.66	-0.0273	0.1289	2.83	-14.79	2.83
ammonia	0	-4.29	-6.41	2.12	-0.0367	0.0681	1.56	-4.86	0.57
methylamine	0	-4.56	-5.23	0.67	-0.0367	0.0645	1.54	-3.69	-0.87
ethylamine	0	-4.50	-5.39	0.89	-0.0370	0.0632	1.50	-3.88	-0.62
butylamine	0	-4.29	-5.56	1.27	-0.0369	0.0623	1.51	-4.06	-0.23
propylamine	0	-4.39	-5.48	1.09	-0.0368	0.0630	1.53	-3.95	-0.44
pentylamine	0	-4.10	-5.70	1.60	-0.0370	0.0626	1.49	-4.22	0.12
dimethylamine	0	-4.29	-3.99	-0.30	-0.0354	0.0638	1.83	-2.17	-2.12
diethylamine	0	-4.07	-3.99	-0.08	-0.0353	0.0608	1.83	-2.16	-1.91
dipropylamine	0	-3.66	-4.15	0.49	-0.0351	0.0605	1.88	-2.26	-1.40
trimethylamine	0	-3.23	-2.69	-0.54	-0.0335	0.0337	2.17	-0.52	-2.71
azetidine	0	-5.56	-4.30	-1.26	-0.0368	0.0618	1.54	-2.76	-2.80
pyrrolidine	0	-5.48	-4.64	-0.84	-0.0367	0.0616	1.55	-3.09	-2.39
piperidine	0	-5.11	-3.64	-1.47	-0.0349	0.0626	1.92	-1.72	-3.39
2-methoxyethanamine	0	-6.55	-8.34	1.79	-0.0354	0.0651	1.81	-6.53	-0.02
1,2-ethanediamine	0	-9.72	-10.20	0.48	-0.0358	0.0651	1.75	-8.45	-1.27
nitromethane	0	-3.95	-8.99	5.04	-0.0222	0.0595	3.37	-5.62	1.67
nitroethane	0	-3.71	-8.54	4.83	-0.0230	0.0553	3.32	-5.22	1.51
1-nitropropane	0	-3.34	-8.51	5.17	-0.0230	0.0546	3.32	-5.18	1.84
2-nitropropane	0	-3.14	-7.86	4.72	-0.0234	0.0524	3.30	-4.56	1.42
1-nitrobutane	0	-3.08	-8.60	5.52	-0.0231	0.0545	3.32	-5.28	2.20
nitrobenzene	0	-4.12	-8.05	3.93	-0.0228	0.0547	3.34	-4.71	0.59
2-methyl-1-nitrobenzene	0	-3.59	-7.74	4.15	-0.0241	0.0520	3.25	-4.49	0.90
pyridine	0	-4.70	-5.79	1.09	-0.0363	0.0492	1.65	-4.13	-0.57
2-methylpyridine	0	-4.63	-5.51	0.88	-0.0366	0.0472	1.59	-3.91	-0.72
3-methylpyridine	0	-4.77	-5.89	1.12	-0.0369	0.0468	1.52	-4.38	-0.39
4-methylpyridine	0	-4.94	-6.07	1.13	-0.0373	0.0455	1.44	-4.63	-0.31
4-ethylpyridine	0	-4.74	-6.12	1.38	-0.0373	0.0457	1.44	-4.68	-0.06
2,4-dimethylpyridine	0	-4.86	-5.78	0.92	-0.0375	0.0438	1.39	-4.38	-0.48

2,5-dimethylpyridine	0	-4.72	-5.59	0.87	-0.0370	0.0456	1.50	-4.09	-0.63
2,6-dimethylpyridine	0	-4.60	-5.25	0.65	-0.0367	0.0468	1.56	-3.69	-0.91
3,4-dimethylpyridine	0	-5.22	-6.28	1.06	-0.0378	0.0448	1.32	-4.96	-0.26
3,5-dimethylpyridine	0	-4.84	-6.00	1.16	-0.0375	0.0457	1.39	-4.61	-0.23
aniline	0	-5.49	-8.26	2.77	-0.0258	0.0805	3.10	-5.17	-0.32
N-methylaniline	0	-4.68	-6.68	2.00	-0.0222	0.0793	3.35	-3.32	-1.36
2-methylaniline	0	-5.56	-7.78	2.22	-0.0266	0.0776	3.03	-4.75	-0.81
3-methylaniline	0	-5.67	-8.20	2.53	-0.0265	0.0796	3.03	-5.16	-0.51
4-methylaniline	0	-5.55	-8.09	2.54	-0.0268	0.0774	3.01	-5.08	-0.47
N-ethylaniline	0	-4.62	-6.60	1.98	-0.0197	0.0807	3.48	-3.13	-1.49
3-aminoaniline	0	-9.92	-13.14	3.22	-0.0267	0.0788	3.02	-10.12	0.20
N,N-dimethylaniline	0	-3.58	-5.10	1.52	-0.0170	0.0394	3.60	-1.50	-2.08
piperazine	0	-7.40	-6.66	-0.74	-0.0346	0.0637	1.97	-4.69	-2.71
N-methylpiperazine	0	-7.77	-5.47	-2.30	-0.0342	0.0643	2.04	-3.43	-4.34
N,N'-dimethylpiperazine	0	-7.58	-4.25	-3.33	-0.0325	0.0337	2.33	-1.92	-5.66
1-methylthymine	0	-10.40	-16.86	6.46	-0.0347	0.1074	1.88	-14.99	4.59
9-methyladenine	0	-13.60	-15.32	1.72	-0.0398	0.0973	0.77	-14.55	0.95
acetamide	0	-9.71	-12.68	2.97	-0.0368	0.0962	1.48	-11.19	1.48
E-N-methylacetamide	0	-10.00	-11.32	1.32	-0.0384	0.0876	1.16	-10.16	0.16
Z-N-methylacetamide	0	-10.00	-10.74	0.74	-0.0386	0.0951	1.08	-9.65	-0.35
benzamide	0	-10.90	-13.02	2.12	-0.0365	0.0960	1.55	-11.46	0.56
2,6-dichlorothiobenzamide	0	-10.81	-14.77	3.96	-0.0242	0.1102	3.16	-11.60	0.79
urea	0	-13.80	-16.26	2.46	-0.0365	0.0934	1.55	-14.71	0.91
1,1-dimethyl-3-phenylurea	0	-9.63	-12.28	2.65	-0.0349	0.0881	1.89	-10.38	0.75
hydrazine	0	-6.26	-9.33	3.07	-0.0348	0.0683	1.93	-7.40	1.14
methylhydrazine	0	-5.31	-8.17	2.86	-0.0345	0.0682	1.98	-6.19	0.88
1,1-dimethylhydrazine	0	-4.48	-6.59	2.11	-0.0348	0.0687	1.94	-4.66	0.18
2-methylpyrazine	0	-5.57	-6.67	1.10	-0.0321	0.0492	2.39	-4.28	-1.29
2-ethylpyrazine	0	-5.51	-6.28	0.77	-0.0322	0.0488	2.37	-3.91	-1.60
morpholine	0	-7.17	-6.80	-0.37	-0.0332	0.0664	2.21	-4.59	-2.58
N-methylmorpholine	0	-6.34	-5.48	-0.86	-0.0315	0.0372	2.48	-3.00	-3.34
acetonitrile	0	-3.89	-8.72	4.83	-0.0317	0.0563	2.44	-6.28	2.39
butanonitrile	0	-3.64	-8.07	4.43	-0.0317	0.0521	2.45	-5.62	1.98
propionitrile	0	-3.85	-8.30	4.45	-0.0319	0.0524	2.43	-5.87	2.02
benzonitrile	0	-4.10	-8.46	4.36	-0.0310	0.0528	2.54	-5.91	1.81

2,6-dichlorobenzonitrile	0	-5.22	-8.92	3.70	-0.0298	0.0569	2.71	-6.21	0.99
3,5-dibromo-4-hydroxybenzonitrile	0	-9.00	-12.15	3.15	-0.0299	0.1083	2.61	-9.54	0.54
trimethylphosphate	0	-8.70	-11.78	3.08	-0.0340	0.0543	2.09	-9.69	0.99
2,2-dichloroethenyl dimethyl phosphate	0	-6.61	-11.25	4.64	-0.0301	0.0671	2.65	-8.60	1.99
phosphine	0	0.60	-1.10	1.70	-0.0079	0.0394	3.72	2.63	-2.03
hydrogen sulfide	0	-0.70	-3.45	2.75	-0.0102	0.0624	3.70	0.25	-0.95
dimethyl sulfide	0	-1.54	-3.73	2.19	-0.0181	0.0428	3.56	-0.17	-1.37
diethyl sulfide	0	-1.43	-3.65	2.22	-0.0190	0.0364	3.53	-0.12	-1.31
dipropyl sulfide	0	-1.27	-3.88	2.61	-0.0193	0.0361	3.52	-0.36	-0.91
bis(2-chloroethyl)sulfide	0	-3.92	-7.83	3.91	-0.0130	0.0499	3.68	-4.15	0.23
dimethyl disulfide	0	-1.83	-4.32	2.49	-0.0122	0.0457	3.69	-0.63	-1.20
diethyl disulfide	0	-1.63	-4.01	2.38	-0.0126	0.0426	3.68	-0.33	-1.30
methanethiol	0	-1.24	-3.59	2.35	-0.0147	0.0553	3.65	0.06	-1.30
ethanethiol	0	-1.30	-3.62	2.32	-0.0151	0.0539	3.64	0.02	-1.32
1-propanethiol	0	-1.05	-3.73	2.68	-0.0152	0.0537	3.64	-0.10	-0.95
thiophene	0	-1.42	-3.83	2.41	-0.0039	0.0532	3.73	-0.10	-1.32
thiophenol	0	-2.55	-5.24	2.69	-0.0087	0.0608	3.71	-1.53	-1.02
thioanisole	0	-2.73	-5.36	2.63	-0.0120	0.0466	3.69	-1.67	-1.06
tetramethylsilane	0	3.04	-1.75	4.79	0.0009	0.0328	3.73	1.99	1.05
acetylene	-1	-76.50	-71.22	-5.28	-0.0621	0.0401	-10.65	-81.87	5.37
acetonitrile	-1	-66.60	-63.59	-3.01	-0.0573	0.0163	-7.04	-70.63	4.03
cyanamide	-1	-72.20	-68.09	-4.11	-0.0576	0.0456	-7.27	-75.36	3.16
aniline	-1	-62.90	-58.14	-4.76	-0.0612	0.0242	-9.94	-68.09	5.19
diphenylamine	-1	-54.60	-50.12	-4.48	-0.0538	0.0281	-4.83	-54.95	0.35
hydrogen cyanide	-1	-70.20	-69.78	-0.42	-0.0561	-0.0333	-6.24	-76.02	5.82
formic acid	-1	-76.20	-68.65	-7.55	-0.0563	0.0104	-6.38	-75.03	-1.17
acetic acid	-1	-77.60	-68.13	-9.47	-0.0580	0.0221	-7.55	-75.67	-1.93
propanoic acid	-1	-76.20	-65.98	-10.22	-0.0582	0.0203	-7.64	-73.62	-2.58
hexanoic acid	-1	-74.60	-65.20	-9.40	-0.0582	0.0273	-7.69	-72.90	-1.70
acrylic acid	-1	-74.00	-66.68	-7.32	-0.0577	0.0334	-7.32	-74.00	0.00
pyruvic acid	-1	-68.50	-66.02	-2.48	-0.0546	0.0359	-5.32	-71.34	2.84
benzoic acid	-1	-71.20	-63.68	-7.52	-0.0570	0.0365	-6.86	-70.53	-0.67
methanol	-1	-95.00	-70.83	-24.17	-0.0697	-0.0087	-18.10	-88.93	-6.07
ethanol	-1	-90.70	-67.30	-23.40	-0.0700	0.0148	-18.46	-85.77	-4.93
1-propanol	-1	-88.30	-66.90	-21.40	-0.0703	0.0211	-18.72	-85.62	-2.68

isopropanol	-1	-86.30	-64.83	-21.47	-0.0695	0.0149	-17.84	-82.67	-3.63
2-butanol	-1	-84.20	-61.67	-22.53	-0.0690	0.0150	-17.24	-78.92	-5.28
t-butanol	-1	-82.30	-63.08	-19.22	-0.0688	0.0153	-17.06	-80.14	-2.16
allyl alcohol	-1	-86.60	-66.69	-19.91	-0.0694	0.0254	-17.69	-84.37	-2.23
benzyl alcohol	-1	-85.10	-62.11	-22.99	-0.0684	0.0320	-16.64	-78.76	-6.34
2-methoxyethanol	-1	-89.40	-68.62	-20.78	-0.0698	0.0292	-18.21	-86.83	-2.57
phenol	-1	-71.90	-59.96	-11.94	-0.0611	0.0254	-9.82	-69.79	-2.11
2-methylphenol	-1	-70.20	-58.16	-12.04	-0.0614	0.0237	-10.07	-68.23	-1.97
3-methylphenol	-1	-71.10	-59.80	-11.30	-0.0614	0.0269	-10.08	-69.88	-1.22
4-methylphenol	-1	-72.00	-59.76	-12.24	-0.0618	0.0252	-10.40	-70.16	-1.84
1,2-ethanediol	-1	-85.30	-72.82	-12.48	-0.0700	0.0940	-18.51	-91.34	6.04
3-hydroxyphenol	-1	-73.80	-63.24	-10.56	-0.0604	0.1021	-9.32	-72.56	-1.24
4-hydroxyphenol	-1	-77.60	-64.97	-12.63	-0.0621	0.1010	-10.76	-75.73	-1.87
methyl hydroperoxide	-1	-93.20	-74.16	-19.04	-0.0704	0.0190	-18.91	-93.06	-0.14
ethyl hydroperoxide	-1	-89.20	-73.68	-15.52	-0.0708	0.0265	-19.30	-92.98	3.78
acetaldehyde	-1	-76.50	-65.23	-11.27	-0.0623	0.0135	-10.81	-76.04	-0.46
acetone	-1	-76.20	-64.05	-12.15	-0.0629	0.0186	-11.34	-75.40	-0.80
3-pentanone	-1	-73.70	-58.69	-15.01	-0.0616	0.0184	-10.23	-68.92	-4.78
water	-1	-104.70	-84.55	-20.15	-0.0754	0.0222	-25.17	-109.71	5.01
hydrogen peroxide	-1	-97.30	-81.85	-15.45	-0.0710	0.0746	-19.56	-101.41	4.11
hydroperoxyl radical	-1	-83.30	-76.08	-7.22	-0.0610	-0.0409	-9.78	-85.86	2.56
2-nitrophenol	-1	-60.10	-57.72	-2.38	-0.0538	0.0365	-4.88	-62.60	2.50
3-nitrophenol	-1	-61.90	-54.62	-7.28	-0.0571	0.0409	-6.92	-61.53	-0.37
4-nitrophenol	-1	-57.80	-52.88	-4.92	-0.0518	0.0387	-3.74	-56.62	-1.18
nitromethane	-1	-76.50	-66.22	-10.28	-0.0551	0.0286	-5.64	-71.86	-4.64
4-nitroaniline	-1	-57.40	-52.95	-4.45	-0.0511	0.0399	-3.41	-56.36	-1.04
acetamide	-1	-80.20	-66.08	-14.12	-0.0590	0.0239	-8.24	-74.33	-5.87
methanethiol	-1	-73.80	-65.62	-8.18	-0.0485	0.0156	-2.18	-67.80	-6.00
ethanethiol	-1	-71.80	-63.21	-8.59	-0.0485	0.0209	-2.16	-65.38	-6.42
1-propanethiol	-1	-70.50	-63.13	-7.37	-0.0486	0.0247	-2.23	-65.36	-5.14
thiophenol	-1	-63.40	-57.31	-6.09	-0.0435	0.0319	-0.27	-57.58	-5.82
hydrogen sulfide	-1	-72.10	-66.96	-5.14	-0.0461	0.0129	-1.17	-68.13	-3.97
dimethyl sulfoxide	-1	-67.70	-61.79	-5.91	-0.0583	0.0286	-7.77	-69.55	1.85
hydrofluoric acid	-1	-104.40	-90.23	-14.17	-0.0784	-0.0784	-29.55	-119.78	15.38
hydrochloric acid	-1	-74.50	-71.25	-3.25	-0.0453	-0.0453	-0.91	-72.16	-2.34

hydrobromic acid	-1	-68.30	-66.25	-2.05	-0.0378	-0.0378	1.32	-64.93	-3.37
chloroform	-1	-54.10	-51.71	-2.39	-0.0407	0.0036	0.60	-51.11	-2.99
trifluoroacetic acid	-1	-59.30	-60.32	1.02	-0.0506	0.0458	-3.18	-63.50	4.20
chloroacetic acid	-1	-69.70	-62.79	-6.91	-0.0534	0.0355	-4.64	-67.43	-2.27
dichloroacetic acid	-1	-62.30	-58.81	-3.49	-0.0505	0.0450	-3.10	-61.92	-0.38
2,2,2-trifluoroethanol	-1	-77.50	-63.32	-14.18	-0.0658	0.0282	-13.98	-77.29	-0.21
1,1,1,3,3,3-hexafluoropropan-2-ol	-1	-65.50	-58.16	-7.34	-0.0611	0.0336	-9.85	-68.01	2.51
2-chlorophenol	-1	-66.10	-57.02	-9.08	-0.0587	0.0323	-7.99	-65.01	-1.09
4-chlorophenol	-1	-66.00	-55.57	-10.43	-0.0593	0.0324	-8.44	-64.00	-2.00
methylamine	1	-76.40	-82.87	6.47	0.0311	0.1423	3.51	-79.35	2.95
n-propylamine	1	-71.50	-77.56	6.06	0.0073	0.1398	3.53	-74.03	2.53
isopropylamine	1	-69.60	-75.76	6.16	0.0070	0.1376	3.54	-72.22	2.62
tert-butylamine	1	-67.30	-73.02	5.72	0.0080	0.1360	3.55	-69.47	2.17
cyclohexanamine	1	-68.70	-72.58	3.88	0.0065	0.1367	3.54	-69.03	0.33
allylamine	1	-72.00	-78.36	6.36	-0.0109	0.1432	3.48	-74.87	2.87
dimethylamine	1	-68.60	-74.29	5.69	0.0293	0.1370	3.54	-70.75	2.15
diethylamine	1	-63.40	-67.88	4.48	0.0086	0.1298	3.58	-64.31	0.91
di-n-propylamine	1	-60.50	-65.65	5.15	0.0097	0.1300	3.57	-62.08	1.58
diallylamine	1	-61.60	-67.36	5.76	-0.0083	0.1325	3.55	-63.80	2.20
trimethylamine	1	-61.10	-66.85	5.75	0.0283	0.1333	3.56	-63.29	2.19
triethylamine	1	-54.60	-58.92	4.32	0.0081	0.1185	3.62	-55.30	0.70
aniline	1	-72.40	-77.93	5.53	0.0070	0.1470	3.49	-74.44	2.04
2-methylaniline	1	-70.30	-75.54	5.24	0.0008	0.1440	3.50	-72.04	1.74
3-methylaniline	1	-69.60	-76.05	6.45	0.0056	0.1472	3.49	-72.56	2.96
4-methylaniline	1	-69.80	-75.97	6.17	0.0065	0.1467	3.49	-72.48	2.68
3-aminoaniline	1	-65.80	-79.00	13.20	-0.0138	0.1458	3.43	-75.57	9.77
N-methylaniline	1	-62.60	-69.46	6.86	0.0067	0.1394	3.53	-65.93	3.33
N-ethylaniline	1	-62.20	-66.46	4.26	0.0070	0.1354	3.55	-62.91	0.71
N,N-dimethylaniline	1	-57.20	-62.13	4.93	0.0070	0.1314	3.57	-58.56	1.36
4-methyl-N,N-dimethylaniline	1	-55.90	-60.52	4.62	0.0064	0.1288	3.58	-56.94	1.04
N,N-diethylaniline	1	-54.00	-57.49	3.49	0.0063	0.1222	3.61	-53.88	-0.12
1-aminonaphthalene	1	-67.40	-74.41	7.01	0.0040	0.1480	3.48	-70.93	3.53
aziridine	1	-70.90	-76.20	5.30	0.0305	0.1443	3.50	-72.70	1.80
azetidine	1	-67.70	-72.02	4.32	0.0188	0.1348	3.55	-68.47	0.77
pyrrolidine	1	-66.00	-69.57	3.57	0.0106	0.1332	3.56	-66.01	0.01

piperidine	1	-64.20	-67.73	3.53	0.0075	0.1350	3.55	-64.18	-0.02
azacycloheptane	1	-63.30	-66.09	2.79	0.0021	0.1347	3.55	-62.54	-0.76
pyrrole	1	-61.40	-67.54	6.14	0.0177	0.1429	3.51	-64.03	2.63
pyridine	1	-61.10	-65.71	4.61	0.0226	0.1452	3.50	-62.21	1.11
quinoline	1	-56.00	-59.69	3.69	0.0104	0.1362	3.55	-56.15	0.15
piperazine	1	-66.00	-70.83	4.83	-0.0238	0.1357	3.09	-67.74	1.74
acetonitrile	1	-75.30	-77.36	2.06	0.0395	0.2104	2.83	-74.52	-0.78
ammonia	1	-85.20	-93.49	8.29	0.0712	0.1507	3.46	-90.02	4.82
hydrazine	1	-84.60	-92.09	7.49	-0.0098	0.1497	3.45	-88.64	4.04
methanol	1	-93.00	-91.27	-1.73	0.0178	0.2111	2.82	-88.45	-4.55
ethanol	1	-88.40	-85.17	-3.23	-0.0015	0.2064	2.89	-82.28	-6.12
dimethyl ether	1	-79.70	-76.65	-3.05	0.0144	0.2015	2.96	-73.68	-6.02
diethyl ether	1	-71.50	-67.97	-3.53	0.0085	0.1844	3.17	-64.80	-6.70
acetone	1	-77.10	-73.64	-3.46	0.0081	0.1834	3.19	-70.46	-6.64
acetophenone	1	-64.50	-61.53	-2.97	0.0036	0.1523	3.45	-58.08	-6.42
water	1	-110.30	-110.49	0.19	0.0229	0.2277	2.54	-107.95	-2.35
4-methoxyaniline	1	-71.20	-76.84	5.64	-0.0193	0.1441	3.29	-73.54	2.34
4-nitroaniline	1	-75.90	-91.43	15.53	-0.0168	0.1500	3.34	-88.09	12.19
morpholine	1	-69.60	-75.06	5.46	-0.0185	0.1390	3.35	-71.71	2.11
acetamide	1	-73.90	-79.88	5.98	0.0017	0.1746	3.27	-76.60	2.70
benzamide	1	-67.20	-71.66	4.46	-0.0008	0.1691	3.32	-68.34	1.14
dimethyl sulfide	1	-64.50	-68.21	3.71	0.0279	0.1065	3.66	-64.55	0.05
dimethyl sulfoxide	1	-67.70	-70.77	3.07	-0.0024	0.1703	3.31	-67.46	-0.24
3-chloroaniline	1	-74.70	-80.86	6.16	-0.0024	0.1483	3.48	-77.38	2.68
4-chloroaniline	1	-74.10	-81.20	7.10	-0.0002	0.1494	3.47	-77.73	3.63
PEARSON			0.99					1.00	