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	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
toluene	–0.66	–4.08	–4.75	–4.75	–5.07	–4.97	–4.25
ethylbenzene	–0.62	–4.58	–5.21	–5.21	–5.26	–5.28	–4.48
phenol	–1.31	–6.87	–8.18	–8.18	–8.36	–8.19	–8.55
o-cresol	–1.34	–7.08	–8.42	–8.42	–8.66	–8.49	–8.57
p-cresol	–1.31	–7.11	–8.43	–8.43	–8.59	–8.48	–9.25
formaldehyde	–2.42	–0.45	–2.86	–2.86	–2.73	–2.80	–3.44
ethanoic acid	–3.27	–3.50	–6.78	–6.78	–6.89	–6.86	–6.65
propanoic acid	–2.90	–4.07	–6.98	–6.98	–7.07	–7.05	–7.09
butanoic acid	–2.83	–4.60	–7.43	–7.43	–7.31	–7.40	–7.74
pentanoic acid	–2.79	–5.15	–7.94	–7.94	–7.82	–7.92	–8.17
hexanoic acid	–2.79	–5.70	–8.49	–8.49	–8.28	–8.42	–8.99
methylamine	–0.22	–3.21	–3.44	–3.44	–3.44	–3.34	–3.95
ethylamine	–0.21	–3.94	–4.15	–4.15	–4.08	–4.09	–4.27
propylamine	–0.19	–4.54	–4.72	–4.72	–4.63	–4.67	–4.88
butylamine	–0.18	–5.09	–5.27	–5.27	–5.12	–5.20	–5.50
diethylamine	–0.27	–4.43	–4.70	–4.70	–4.40	–4.67	–5.30
aniline	–0.88	–6.01	–6.89	–6.89	–7.27	–7.23	–6.44
ammonia	–0.17	–3.15	–3.32	–3.32	–3.51	–3.11	–3.13
p-bromophenol	–1.57	–8.18	–9.75	–9.70	–9.96	–9.69	–10.62
			Solvent: hexanol				
benzene	–0.61	–3.82	–4.42	–4.42	–4.68	–4.58	–3.68
toluene	–0.65	–4.09	–4.74	–4.74	–5.02	–4.93	–4.27
ethylbenzene	–0.61	–4.59	–5.20	–5.20	–5.21	–5.25	–4.54
phenol	–1.29	–6.88	–8.17	–8.17	–8.29	–8.15	–8.76
o-cresol	–1.31	–7.10	–8.41	–8.41	–8.60	–8.45	–8.76
m-cresol	–1.32	–7.12	–8.44	–8.44	–8.60	–8.48	–8.42
p-cresol	–1.29	–7.12	–8.42	–8.42	–8.53	–8.44	–9.21
formaldehyde	–2.37	–0.44	–2.81	–2.81	–2.65	–2.73	–3.42
ethanoic acid	–3.21	–3.50	–6.71	–6.71	–6.81	–6.78	–6.51

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
ethylamine	–0.21	–3.94	–4.14	–4.14	–4.08	–4.09	–4.20
propylamine	–0.18	–4.54	–4.72	–4.72	–4.62	–4.68	–4.83
butylamine	–0.18	–5.10	–5.27	–5.27	–5.12	–5.20	–5.40
p-bromophenol	–1.54	–8.20	–9.74	–9.69	–9.90	–9.66	–10.51
Solvent: heptanol							
benzene	–0.60	–3.81	–4.42	–4.42	–4.63	–4.55	–3.73
toluene	–0.64	–4.09	–4.73	–4.73	–4.96	–4.90	–4.33
ethylbenzene	–0.61	–4.59	–5.19	–5.19	–5.16	–5.21	–4.58
phenol	–1.27	–6.88	–8.15	–8.15	–8.24	–8.11	–8.69
o-cresol	–1.30	–7.09	–8.39	–8.39	–8.54	–8.41	–8.78
p-cresol	–1.28	–7.12	–8.40	–8.40	–8.47	–8.40	–9.16
ethanoic acid	–3.17	–3.50	–6.67	–6.67	–6.75	–6.72	–6.70
ethylamine	–0.20	–3.93	–4.14	–4.14	–4.06	–4.08	–4.15
propylamine	–0.18	–4.54	–4.72	–4.72	–4.61	–4.67	–4.80
butylamine	–0.18	–5.09	–5.26	–5.26	–5.10	–5.19	–5.33
p-bromophenol	–1.53	–8.20	–9.73	–9.67	–9.85	–9.62	–10.49
Solvent: octanol							
methane	–0.01	0.47	0.47	0.47	0.71	0.60	0.51
ethane	0.00	–0.62	–0.62	–0.62	–0.48	–0.50	–0.64
propane	0.00	–1.23	–1.23	–1.23	–1.10	–1.11	–1.26
n-butane	0.00	–1.78	–1.78	–1.78	–1.60	–1.63	–1.86
n-pentane	0.00	–2.33	–2.33	–2.33	–2.09	–2.15	–2.45
n-hexane	0.00	–2.88	–2.88	–2.88	–2.56	–2.66	–3.01
n-heptane	0.00	–3.43	–3.43	–3.43	–3.04	–3.17	–3.74
n-octane	0.00	–3.98	–3.98	–3.98	–3.51	–3.68	–4.18
2-methylpropane	–0.01	–1.49	–1.50	–1.50	–1.36	–1.38	–1.45
2,2-dimethylpropane	–0.02	–1.58	–1.60	–1.60	–1.51	–1.51	–1.74
cyclopropane	–0.07	–2.22	–2.30	–2.30	–2.08	–2.12	–1.60
cyclopentane	–0.01	–2.93	–2.94	–2.94	–2.94	–2.84	–2.65

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				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
cyclohexane	0.00	–3.40	–3.40	–3.40	–3.43	–3.32	–3.46
methylcyclohexane	–0.01	–3.56	–3.56	–3.56	–3.45	–3.42	–3.21
ethene	–0.09	–0.26	–0.35	–0.35	0.07	–0.10	–0.27
propene	–0.13	–1.06	–1.19	–1.19	–0.88	–1.00	–1.14
s-trans-1,3-butadiene	–0.26	–1.49	–1.75	–1.75	–1.11	–1.37	–2.10
2-methylpropene	–0.19	–1.41	–1.60	–1.60	–1.42	–1.48	–2.03
1-butene	–0.12	–1.61	–1.73	–1.73	–1.28	–1.47	–1.89
1-hexene	–0.11	–2.71	–2.81	–2.81	–2.21	–2.46	–2.94
ethyne	–1.32	0.67	–0.64	–0.64	–0.57	–0.60	–0.51
propyne	–1.47	–0.46	–1.93	–1.93	–2.28	–2.20	–1.59
1-pentyne	–1.35	–1.56	–2.90	–2.90	–2.81	–2.89	–2.79
1-hexyne	–1.33	–2.10	–3.43	–3.43	–3.30	–3.40	–3.43
benzene	–0.59	–3.81	–4.40	–4.40	–4.57	–4.51	–3.72
toluene	–0.63	–4.08	–4.71	–4.71	–4.89	–4.85	–4.55
ethylbenzene	–0.60	–4.58	–5.17	–5.17	–5.09	–5.17	–5.08
o-xylene	–0.69	–4.37	–5.06	–5.06	–5.34	–5.27	–5.07
m-xylene	–0.67	–4.35	–5.02	–5.02	–5.23	–5.20	–5.25
p-xylene	–0.66	–4.35	–5.01	–5.01	–5.20	–5.18	–5.19
naphthalene	–1.07	–6.19	–7.26	–7.26	–7.65	–7.52	–6.97
anthracene	–1.48	–8.56	–10.04	–10.04	–10.43	–10.34	–10.47
methanol	–1.14	–3.29	–4.43	–4.43	–4.43	–4.40	–3.87
ethanol	–1.00	–4.15	–5.15	–5.15	–5.26	–5.18	–4.36
1,2-ethanediol	–1.71	–6.30	–8.01	–8.01	–8.15	–8.23	–7.44
1-propanol	–0.97	–4.73	–5.70	–5.70	–5.65	–5.65	–5.02
2-propanol	–0.94	–4.55	–5.50	–5.50	–5.26	–5.36	–4.62
1-butanol	–0.96	–5.30	–6.26	–6.26	–6.04	–6.13	–5.71
2-methyl-2-propanol	–0.85	–4.67	–5.52	–5.52	–5.48	–5.47	–4.78
1-pentanol	–0.95	–5.85	–6.80	–6.80	–6.50	–6.63	–6.40
phenol	–1.25	–6.87	–8.13	–8.13	–8.16	–8.06	–8.69

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Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
1-hexanol	–1.00	–6.24	–7.24	–7.24	–6.89	–7.09	–7.06
o-cresol	–1.28	–7.09	–8.36	–8.36	–8.45	–8.35	–8.49
m-cresol	–1.29	–7.11	–8.39	–8.39	–8.46	–8.38	–8.20
p-cresol	–1.26	–7.11	–8.37	–8.37	–8.39	–8.35	–8.84
1-heptanol	–1.00	–6.79	–7.79	–7.79	–7.37	–7.61	–7.75
1-octanol	–0.95	–7.49	–8.44	–8.44	–7.95	–8.16	–8.13
1-decanol	–0.93	–8.58	–9.51	–9.51	–9.01	–9.22	–9.88
dimethyl ether	–1.18	–0.59	–1.77	–1.77	–1.75	–1.66	–2.06
tetrahydrofuran	–1.45	–2.78	–4.23	–4.23	–4.25	–4.11	–3.93
1,4-dioxane	–2.26	–2.76	–5.02	–5.02	–5.08	–4.98	–4.89
diethyl ether	–0.97	–2.17	–3.14	–3.14	–3.15	–3.09	–2.89
methyl propyl ether	–1.03	–1.96	–2.98	–2.98	–2.85	–2.86	–3.63
methyl isopropyl ether	–1.03	–1.79	–2.82	–2.82	–2.74	–2.72	–4.64
1,2-dimethoxyethane	–1.66	–2.12	–3.78	–3.78	–3.66	–3.72	–4.55
t-butyl methyl ether	–1.00	–1.92	–2.91	–2.91	–2.82	–2.81	–3.49
anisole	–1.48	–4.16	–5.64	–5.64	–5.69	–5.49	–5.47
tetrahydropyran	–1.07	–3.31	–4.38	–4.38	–4.46	–4.34	–4.21
ethyl phenyl ether	–1.34	–4.91	–6.25	–6.25	–6.18	–6.08	–5.65
formaldehyde	–2.29	–0.42	–2.71	–2.71	–2.52	–2.61	–3.23
propanal	–1.90	–2.18	–4.08	–4.08	–4.19	–4.22	–4.13
butanal	–1.88	–2.70	–4.58	–4.58	–4.53	–4.63	–4.62
benzaldehyde	–2.26	–5.00	–7.26	–7.26	–7.05	–7.14	–6.13
propanone	–2.14	–2.29	–4.43	–4.43	–4.52	–4.53	–3.15
butanone	–1.91	–2.81	–4.72	–4.72	–4.91	–4.88	–3.78
cyclopentanone	–1.86	–4.00	–5.86	–5.86	–5.77	–5.81	–5.01
2-pentanone	–1.90	–3.33	–5.22	–5.22	–5.23	–5.28	–4.35
3-pentanone	–1.69	–3.34	–5.03	–5.03	–5.27	–5.23	–4.36
2-hexanone	–1.75	–3.90	–5.66	–5.66	–5.67	–5.69	–5.02
3,3-dimethylbutanone	–1.78	–3.05	–4.83	–4.83	–4.90	–4.88	–4.53

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				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
2-heptanone	–1.87	–4.43	–6.30	–6.30	–6.20	–6.29	–5.65
methyl phenyl ketone	–2.38	–5.60	–7.98	–7.98	–7.79	–7.82	–6.74
2-octanone	–1.86	–4.97	–6.83	–6.83	–6.69	–6.80	–6.38
ethanoic acid	–3.12	–3.49	–6.60	–6.60	–6.66	–6.64	–6.35
propanoic acid	–2.77	–4.05	–6.82	–6.82	–6.85	–6.85	–6.86
butanoic acid	–2.70	–4.58	–7.28	–7.28	–7.10	–7.20	–7.58
pentanoic acid	–2.66	–5.13	–7.79	–7.79	–7.61	–7.72	–8.22
hexanoic acid	–2.65	–5.68	–8.33	–8.33	–8.07	–8.22	–8.82
methyl methanoate	–3.07	0.02	–3.05	–3.05	–3.12	–3.09	–2.82
methyl ethanoate	–2.97	–0.94	–3.90	–3.90	–4.05	–3.88	–3.54
methyl propanoate	–2.67	–1.50	–4.17	–4.17	–4.28	–4.13	–4.06
ethyl ethanoate	–2.90	–1.73	–4.63	–4.63	–4.65	–4.55	–4.06
methyl butanoate	–2.61	–2.03	–4.64	–4.64	–4.53	–4.49	–4.59
propyl ethanoate	–2.84	–2.30	–5.13	–5.13	–5.03	–5.02	–4.55
methyl pentanoate	–2.57	–2.58	–5.15	–5.15	–5.02	–5.00	–5.13
butyl ethanoate	–2.80	–2.84	–5.65	–5.65	–5.46	–5.51	–4.96
methyl benzoate	–2.98	–4.24	–7.21	–7.21	–6.65	–6.68	–7.26
2-propen-1-ol	–1.00	–4.55	–5.54	–5.54	–5.02	–5.23	–5.27
2-methoxyethanol	–1.73	–4.91	–6.64	–6.64	–6.45	–6.57	–5.83
m-hydroxybenzaldehyde	–2.75	–8.07	–10.82	–10.82	–10.37	–10.52	–11.39
p-hydroxybenzaldehyde	–2.92	–8.05	–10.97	–10.97	–10.58	–10.70	–12.36
water	–1.33	–4.38	–5.71	–5.71	–5.85	–5.77	–4.43
hydrogen	0.00	1.69	1.69	1.69	1.64	1.67	1.76
methylamine	–0.21	–3.21	–3.42	–3.42	–3.40	–3.33	–3.78
ethylamine	–0.20	–3.93	–4.13	–4.13	–4.05	–4.08	–4.09
propylamine	–0.18	–4.53	–4.70	–4.70	–4.59	–4.65	–4.77
trimethylamine	–0.42	–2.90	–3.33	–3.33	–3.39	–3.39	–3.60
piperazine	–0.47	–7.70	–8.17	–8.17	–8.48	–8.48	–5.80
butylamine	–0.17	–5.08	–5.25	–5.25	–5.08	–5.18	–5.35

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Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
diethylamine	–0.26	–4.41	–4.67	–4.67	–4.35	–4.64	–4.75
piperidine	–0.23	–5.63	–5.86	–5.86	–5.88	–6.00	–6.27
dipropylamine	–0.20	–5.70	–5.90	–5.90	–5.46	–5.88	–6.02
pyridine	–1.21	–4.06	–5.27	–5.27	–5.42	–5.16	–5.34
2-methylpyrazine	–1.69	–4.78	–6.47	–6.47	–6.83	–6.31	–5.87
aniline	–0.84	–6.02	–6.86	–6.86	–7.09	–7.11	–6.71
2-methylpyridine	–1.29	–4.52	–5.81	–5.81	–6.16	–5.78	–6.14
3-methylpyridine	–1.19	–4.33	–5.52	–5.52	–5.71	–5.50	–6.40
4-methylpyridine	–1.22	–4.34	–5.56	–5.56	–5.78	–5.55	–6.60
2-ethylpyrazine	–1.56	–5.30	–6.86	–6.86	–7.01	–6.65	–6.40
ethanonitrile	–1.74	–1.34	–3.08	–3.08	–3.13	–3.72	–3.15
propanonitrile	–1.51	–1.91	–3.42	–3.42	–3.31	–3.89	–3.66
butanonitrile	–1.40	–2.46	–3.86	–3.86	–3.54	–4.19	–4.25
benzonitrile	–1.57	–4.76	–6.33	–6.33	–5.65	–6.12	–6.09
nitroethane	–5.80	1.47	–4.33	–4.33	–4.78	–4.42	–3.93
1-nitropropane	–5.46	0.80	–4.65	–4.65	–4.89	–4.90	–4.44
2-nitropropane	–5.25	1.02	–4.22	–4.22	–4.76	–4.17	–4.23
1-nitrobutane	–5.34	0.26	–5.09	–5.09	–5.34	–5.36	–5.11
nitrobenzene	–5.04	–1.28	–6.32	–6.32	–5.55	–6.08	–6.63
2-methyl-1-nitrobenzene	–4.73	–1.72	–6.45	–6.45	–5.87	–6.12	–6.80
1,1-dimethyl-3-phenylurea	–3.44	–7.14	–10.57	–10.57	–10.02	–11.04	–13.12
9-methyladenine	–5.04	–8.95	–13.99	–13.99	–13.78	–13.75	–13.56
morpholine	–1.34	–5.46	–6.80	–6.80	–6.97	–6.99	–5.99
3-ethyl-2-methoxypyrazine	–2.24	–5.55	–7.79	–7.79	–7.80	–7.43	–6.85
hydrazine	–0.19	–7.96	–8.15	–8.15	–8.21	–8.13	–6.48
1-propanethiol	–0.13	–2.58	–2.71	–2.83	–2.56	–2.70	–3.52
thiophenol	–1.04	–4.92	–5.96	–6.07	–5.92	–5.98	–5.99
thiophene	–2.23	–3.43	–5.66	–4.93	–5.32	–4.76	–3.89
diethyl sulfide	–0.13	–3.09	–3.22	–3.42	–3.19	–3.38	–4.09

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				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
thioanisole	–0.93	–5.22	–6.15	–6.39	–6.35	–6.54	–6.47
dimethyl disulfide	–0.41	–3.93	–4.34	–4.41	–4.40	–4.50	–4.24
1,1-difluoroethane	–3.17	0.59	–2.58	–2.63	–2.10	–1.37	–1.13
fluorobenzene	–1.80	–2.99	–4.79	–4.81	–4.16	–4.28	–3.87
dichloromethane	–1.44	–1.71	–3.16	–3.62	–3.52	–2.23	–3.07
trichloromethane	–0.73	–2.71	–3.44	–3.64	–3.99	–3.12	–3.81
chloroethane	–1.37	–1.51	–2.88	–3.18	–2.84	–2.08	–2.58
1,1,1-trichloroethane	–1.06	–3.14	–4.20	–4.33	–4.71	–3.70	–3.69
1,1,2-trichloroethane	–1.57	–3.23	–4.80	–5.26	–5.24	–3.84	–4.53
1-chloropropane	–1.23	–2.10	–3.33	–3.61	–3.14	–2.52	–3.06
2-chloropropane	–1.31	–1.96	–3.27	–3.54	–3.24	–2.53	–2.84
Z-1,2-dichloroethene	–0.97	–1.94	–2.91	–3.42	–3.20	–2.27	–3.71
E-1,2-dichloroethene	–0.54	–1.95	–2.49	–2.71	–2.25	–2.14	–3.61
trichloroethene	–0.41	–2.77	–3.18	–3.32	–3.20	–3.28	–3.75
chlorobenzene	–0.96	–4.41	–5.38	–5.48	–5.24	–5.25	–5.00
o-dichlorobenzene	–1.33	–4.96	–6.29	–6.55	–6.17	–6.14	–6.01
p-dichlorobenzene	–0.92	–5.01	–5.93	–6.09	–5.47	–5.82	–5.67
2,2'-dichlorobiphenyl	–1.89	–8.40	–10.28	–10.45	–9.51	–9.45	–9.41
2,3-dichlorobiphenyl	–1.58	–8.41	–9.99	–10.17	–9.12	–9.44	–9.23
2,2',3'-trichlorobiphenyl	–2.10	–8.93	–11.03	–11.33	–10.17	–10.14	–9.12
bromomethane	–1.00	–1.42	–2.42	–2.73	–1.98	–2.39	–2.43
dibromomethane	–0.61	–3.26	–3.87	–4.29	–3.86	–4.01	–4.18
tribromomethane	–0.16	–4.99	–5.15	–5.24	–5.51	–5.39	–5.62
bromoethane	–0.94	–2.28	–3.23	–3.50	–2.85	–3.34	–2.90
1-bromopropane	–0.85	–2.86	–3.71	–3.96	–3.23	–3.67	–3.42
2-bromopropane	–0.90	–2.71	–3.62	–3.85	–3.27	–3.81	–3.40
3-bromo-propene	–0.86	–2.65	–3.52	–3.72	–2.79	–3.29	–3.30
1-bromobutane	–0.81	–3.41	–4.22	–4.46	–3.70	–4.16	–4.16
1-bromopentane	–0.80	–3.96	–4.76	–5.00	–4.17	–4.66	–4.68

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
bromobenzene	–0.86	–5.16	–6.02	–6.01	–6.08	–5.93	–5.46
p-dibromobenzene	–0.75	–6.51	–7.25	–7.22	–7.20	–7.09	–7.47
bromotoluene	–1.40	–5.55	–6.95	–7.14	–6.81	–7.10	–6.36
diiodomethane	–0.07	–4.68	–4.75	–4.86	–4.98	–4.97	–5.63
iodomethane	–0.52	–2.12	–2.64	–2.34	–2.23	–3.38	–3.07
iodoethane	–0.50	–2.99	–3.48	–3.21	–3.15	–4.43	–3.45
2-iodopropane	–0.48	–3.41	–3.89	–3.64	–3.58	–4.95	–4.40
iodobenzene	–0.80	–5.86	–6.66	–6.78	–6.90	–6.11	–6.18
bromotrifluoromethane	–0.81	0.02	–0.79	–0.60	–0.96	–0.96	–0.75
chlorodifluoromethane	–2.58	0.33	–2.25	–2.43	–2.42	–1.24	–1.97
difluorodichloromethane	–0.40	–0.71	–1.11	–0.95	–1.34	–1.84	–1.25
fluorotrichloromethane	–0.22	–2.17	–2.39	–2.14	–2.69	–3.07	–2.63
tetrafluoromethane	–1.10	2.31	1.21	1.12	1.14	1.09	1.50
1-Br-1-Cl-2,2,2-triFethane	–1.33	–1.25	–2.58	–2.76	–3.01	–2.74	–3.27
tetrachloroethene	–0.05	–3.53	–3.59	–3.21	–3.41	–4.46	–4.24
1,1,2-triCl-1,2,2-triFethane	–0.72	–1.34	–2.06	–1.65	–2.35	–3.60	–2.54
2,2,2-trifluoroethanol	–3.75	–2.28	–6.03	–6.10	–5.90	–5.46	–4.81
1,1-diCl-2,2-diFethyl methyl ether	–2.12	–1.68	–3.80	–3.85	–4.32	–3.68	–4.02
1,1,1-triFpropan-2-ol	–2.99	–2.54	–5.53	–5.60	–5.25	–4.92	–5.12
1,1,1,3,3,3-hexaFpropan-2-ol	–3.86	–0.57	–4.42	–4.56	–4.05	–3.70	–5.76
p-bromophenol	–1.50	–8.20	–9.70	–9.64	–9.77	–9.57	–10.59
2,6-dichlorobenzonitrile	–2.14	–5.97	–8.11	–8.46	–7.60	–7.71	–9.18
4-amino-3,5,6-triClpyridine-2-carboxylic acid	–3.86	–10.73	–14.60	–14.37	–13.75	–15.80	–12.37
			Solvent: nonanol				
benzene	–0.58	–3.79	–4.37	–4.37	–4.48	–4.45	–3.82
toluene	–0.62	–4.06	–4.68	–4.68	–4.80	–4.79	–4.34
ethylbenzene	–0.58	–4.55	–5.13	–5.13	–5.00	–5.10	–4.61
phenol	–1.23	–6.86	–8.09	–8.09	–8.06	–7.99	–8.61

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
2-methoxyethanol	–1.70	–4.89	–6.58	–6.58	–6.37	–6.51	–5.61
ethylamine	–0.20	–3.91	–4.11	–4.11	–4.02	–4.06	–4.02
propylamine	–0.17	–4.51	–4.68	–4.68	–4.56	–4.63	–4.66
butylamine	–0.17	–5.05	–5.22	–5.22	–5.05	–5.15	–5.22
p-bromophenol	–1.47	–8.18	–9.65	–9.59	–9.66	–9.49	–10.36
Solvent: decanol							
phenol	–1.20	–6.85	–8.05	–8.05	–7.96	–7.92	–8.58
o-cresol	–1.22	–7.05	–8.28	–8.28	–8.24	–8.20	–8.58
m-cresol	–1.24	–7.07	–8.31	–8.31	–8.24	–8.23	–8.01
p-cresol	–1.21	–7.08	–8.29	–8.29	–8.18	–8.19	–8.91
2-methoxyethanol	–1.66	–4.87	–6.53	–6.53	–6.30	–6.45	–5.41
ethylamine	–0.19	–3.90	–4.09	–4.09	–4.00	–4.04	–3.91
propylamine	–0.17	–4.49	–4.67	–4.67	–4.54	–4.62	–4.59
butylamine	–0.17	–5.04	–5.20	–5.20	–5.02	–5.13	–5.15
chlorobenzene	–0.92	–4.38	–5.30	–5.40	–5.07	–5.13	–4.83
p-bromophenol	–1.44	–8.17	–9.61	–9.55	–9.56	–9.42	–10.32
Solvent: benzylalcohol							
n-octane	0.00	–4.22	–4.22	–4.22	–3.80	–3.95	–3.77
toluene	–0.65	–4.45	–5.09	–5.09	–5.18	–5.20	–4.46
ethanol	–1.02	–4.36	–5.38	–5.38	–5.47	–5.42	–4.84
1,4-dioxane	–2.31	–2.89	–5.20	–5.20	–5.25	–5.20	–5.39
formaldehyde	–2.35	–0.39	–2.74	–2.74	–2.51	–2.59	–3.48
butanone	–1.96	–2.94	–4.91	–4.91	–5.09	–5.04	–4.57
ethanoic acid	–3.19	–3.76	–6.96	–6.96	–6.98	–6.97	–6.96
Solvent: *m*-cresol							
n-octane	0.00	–3.95	–3.95	–3.95	–3.48	–3.63	–4.02
toluene	–0.65	–3.90	–4.55	–4.55	–4.79	–4.72	–4.58
ethanol	–1.03	–4.35	–5.38	–5.38	–5.54	–5.44	–5.58
1,4-dioxane	–2.33	–2.91	–5.24	–5.24	–5.26	–5.21	–6.82
butanone	–1.98	–2.93	–4.91	–4.91	–5.14	–5.15	–5.98

Solute	SM5.2R/MD// HF/MIDI! ΔG_{EP}	SM5.2R/MD// HF/MIDI! G_{CDS}	SM5.2R/MD// HF/MIDI! ΔG^o_S	SM5.2R//HF/MIDI! MNDO ΔG^o_S	SM5.2R//HF/MIDI! AM1 ΔG^o_S	SM5.2R//HF/MIDI! PM3 ΔG^o_S	Expt ΔG^o_S
Solvent: butanone							
n-octane	0.00	–4.54	–4.54	–4.54	–4.23	–4.33	–4.64
toluene	–0.67	–4.75	–5.42	–5.42	–5.95	–5.76	–5.06
ethanol	–1.06	–3.34	–4.39	–4.39	–4.55	–4.44	–4.46
1,4-dioxane	–2.40	–2.83	–5.22	–5.22	–5.42	–5.19	–5.02
formaldehyde	–2.46	–0.25	–2.70	–2.70	–2.59	–2.63	–1.77
ethanoic acid	–3.32	–3.27	–6.59	–6.59	–6.73	–6.71	–6.88
propanoic acid	–2.95	–3.88	–6.83	–6.83	–6.96	–6.95	–7.05
butanoic acid	–2.87	–4.46	–7.34	–7.34	–7.26	–7.35	–7.34
pentanoic acid	–2.83	–5.06	–7.90	–7.90	–7.83	–7.93	–7.54
hexanoic acid	–2.83	–5.67	–8.49	–8.49	–8.36	–8.49	–8.07
Solvent: 4-methyl-2-pentanone							
naphthalene	–1.11	–7.22	–8.34	–8.34	–9.12	–8.82	–7.45
phenol	–1.29	–6.56	–7.85	–7.85	–8.08	–7.89	–9.38
m-cresol	–1.33	–6.88	–8.20	–8.20	–8.48	–8.31	–8.79
ethanoic acid	–3.22	–3.32	–6.54	–6.54	–6.66	–6.63	–6.33
propanoic acid	–2.86	–3.95	–6.81	–6.81	–6.91	–6.90	–6.85
butanoic acid	–2.79	–4.55	–7.33	–7.33	–7.24	–7.33	–7.44
methylamine	–0.22	–2.34	–2.56	–2.56	–2.52	–2.39	–4.14
trimethylamine	–0.43	–2.09	–2.53	–2.53	–2.77	–2.55	–2.86
diethylamine	–0.27	–3.58	–3.84	–3.84	–3.55	–3.73	–3.63
pyridine	–1.25	–4.00	–5.25	–5.25	–5.74	–5.27	–5.33
aniline	–0.86	–6.08	–6.94	–6.94	–7.38	–7.30	–7.54
ammonia	–0.17	–2.40	–2.56	–2.56	–2.62	–2.29	–2.52
Solvent: cyclohexanone							
n-octane	0.00	–4.06	–4.06	–4.06	–3.61	–3.79	–4.57
toluene	–0.66	–4.55	–5.21	–5.21	–5.50	–5.43	–5.05
ethanol	–1.05	–3.29	–4.34	–4.34	–4.40	–4.34	–4.41
1,4-dioxane	–2.37	–2.56	–4.93	–4.93	–5.01	–4.88	–4.95

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
butanone	–2.02	–2.53	–4.55	–4.55	–4.76	–4.70	–4.42
ethanoic acid	–3.28	–3.22	–6.50	–6.50	–6.52	–6.54	–6.43
propanoic acid	–2.91	–3.79	–6.70	–6.70	–6.70	–6.74	–7.18
Solvent: acetophenone							
n-octane	0.00	–4.46	–4.47	–4.47	–4.06	–4.21	–4.24
toluene	–0.67	–4.84	–5.51	–5.51	–5.85	–5.76	–4.90
ethanol	–1.05	–3.22	–4.28	–4.28	–4.36	–4.30	–4.12
1,4-dioxane	–2.39	–2.82	–5.21	–5.21	–5.26	–5.17	–5.03
butanone	–2.05	–2.73	–4.77	–4.77	–5.00	–4.96	–4.39
ethanoic acid	–3.31	–3.12	–6.43	–6.43	–6.49	–6.50	–6.20
Solvent: ethylacetate							
n-octane	0.00	–4.60	–4.60	–4.60	–4.32	–4.41	–4.72
toluene	–0.58	–4.74	–5.32	–5.32	–5.56	–5.50	–5.05
methanol	–1.04	–2.27	–3.31	–3.31	–3.27	–3.26	–3.37
ethanol	–0.92	–3.19	–4.10	–4.10	–4.18	–4.12	–4.24
1,2-ethanediol	–1.57	–4.87	–6.44	–6.44	–6.52	–6.65	–6.82
1-propanol	–0.89	–3.82	–4.71	–4.71	–4.66	–4.67	–4.90
1-butanol	–0.88	–4.45	–5.33	–5.33	–5.14	–5.22	–5.77
1-pentanol	–0.88	–5.06	–5.93	–5.93	–5.69	–5.79	–6.13
phenol	–1.15	–6.27	–7.42	–7.42	–7.45	–7.36	–8.70
1-hexanol	–0.92	–5.56	–6.48	–6.48	–6.21	–6.37	–6.92
1-heptanol	–0.92	–6.17	–7.09	–7.09	–6.77	–6.95	–7.56
1-octanol	–0.87	–6.88	–7.75	–7.75	–7.38	–7.54	–8.41
1,4-dioxane	–2.08	–2.87	–4.94	–4.94	–5.01	–4.92	–5.03
ethanoic acid	–2.84	–3.11	–5.95	–5.95	–5.98	–5.97	–6.46
propanoic acid	–2.52	–3.73	–6.25	–6.25	–6.27	–6.27	–6.95
butanoic acid	–2.45	–4.32	–6.77	–6.77	–6.62	–6.71	–7.34
water	–1.22	–2.23	–3.45	–3.45	–3.48	–3.46	–4.26

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
Solvent: butylacetate							
naphthalene	–0.93	–7.10	–8.02	–8.02	–8.24	–8.19	–7.59
methanol	–1.00	–2.26	–3.26	–3.26	–3.18	–3.20	–3.04
ethanol	–0.87	–3.19	–4.06	–4.06	–4.10	–4.07	–3.97
1,2-ethanediol	–1.50	–4.88	–6.38	–6.38	–6.41	–6.57	–6.27
1-propanol	–0.85	–3.82	–4.67	–4.67	–4.59	–4.62	–4.52
1-butanol	–0.84	–4.46	–5.30	–5.30	–5.08	–5.18	–5.23
1-pentanol	–0.84	–5.07	–5.90	–5.90	–5.63	–5.75	–5.78
phenol	–1.09	–6.30	–7.40	–7.40	–7.29	–7.26	–8.96
1-hexanol	–0.88	–5.57	–6.45	–6.45	–6.15	–6.33	–6.62
o-cresol	–1.11	–6.61	–7.72	–7.72	–7.68	–7.64	–8.90
m-cresol	–1.13	–6.62	–7.74	–7.74	–7.67	–7.66	–8.44
p-cresol	–1.10	–6.62	–7.72	–7.72	–7.62	–7.63	–9.28
1-heptanol	–0.88	–6.18	–7.06	–7.06	–6.71	–6.91	–7.14
1-octanol	–0.83	–6.89	–7.72	–7.72	–7.33	–7.50	–8.17
ethanoic acid	–2.70	–3.10	–5.80	–5.80	–5.78	–5.79	–6.11
water	–1.17	–2.21	–3.38	–3.38	–3.37	–3.36	–4.13
pyridine	–1.05	–3.96	–5.01	–5.01	–5.19	–4.92	–5.31
aniline	–0.73	–5.90	–6.64	–6.64	–6.74	–6.79	–7.30
p-bromophenol	–1.31	–7.57	–8.88	–8.82	–8.82	–8.70	–10.57
Solvent: butyl ether							
n-octane	0.00	–4.79	–4.79	–4.79	–4.57	–4.62	–5.24
toluene	–0.45	–4.89	–5.34	–5.34	–5.10	–5.24	–4.87
ethanol	–0.72	–3.26	–3.98	–3.98	–3.94	–3.96	–3.51
1,4-dioxane	–1.64	–2.98	–4.62	–4.62	–4.49	–4.64	–4.37
butanone	–1.29	–2.90	–4.20	–4.20	–4.15	–4.12	–3.78
ethanoic acid	–2.19	–3.18	–5.37	–5.37	–5.23	–5.26	–5.21
propanoic acid	–1.95	–3.82	–5.77	–5.77	–5.63	–5.66	–6.11
diethylamine	–0.19	–3.62	–3.81	–3.81	–3.52	–3.76	–3.80
pyridine	–0.85	–4.06	–4.92	–4.92	–4.79	–4.74	–4.65

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
2-methylpyrazine	–1.20	–4.04	–5.25	–5.25	–5.39	–5.13	–5.12
2-methylpyridine	–0.91	–4.51	–5.42	–5.42	–5.40	–5.29	–5.20
2-ethylpyrazine	–1.11	–4.64	–5.75	–5.75	–5.75	–5.60	–5.87
Solvent: tetrahydrofuran							
n-octane	0.00	–4.51	–4.51	–4.51	–4.19	–4.30	–5.39
toluene	–0.60	–4.74	–5.34	–5.34	–5.60	–5.53	–5.50
ethanol	–0.96	–3.24	–4.20	–4.20	–4.27	–4.21	–4.56
1,4-dioxane	–2.17	–2.82	–4.99	–4.99	–5.05	–4.96	–5.17
butanone	–1.81	–2.76	–4.57	–4.57	–4.75	–4.69	–4.54
Solvent: *iso*-propyl ether							
n-octane	0.00	–5.04	–5.04	–5.04	–4.89	–4.90	–5.38
toluene	–0.50	–4.99	–5.49	–5.49	–5.57	–5.56	–4.91
naphthalene	–0.84	–7.33	–8.17	–8.17	–8.28	–8.26	–7.24
ethanol	–0.80	–3.25	–4.05	–4.05	–4.10	–4.06	–3.90
phenol	–1.00	–6.38	–7.38	–7.38	–7.24	–7.23	–8.35
1,4-dioxane	–1.81	–3.12	–4.93	–4.93	–4.95	–4.95	–4.42
formaldehyde	–1.76	–0.34	–2.10	–2.10	–1.83	–1.91	–1.04
butanone	–1.46	–3.03	–4.49	–4.49	–4.60	–4.53	–3.96
ethanoic acid	–2.45	–3.16	–5.61	–5.61	–5.60	–5.59	–5.73
propanoic acid	–2.17	–3.83	–6.00	–6.00	–6.00	–5.98	–6.37
butanoic acid	–2.12	–4.46	–6.58	–6.58	–6.45	–6.50	–6.85
pentanoic acid	–2.09	–5.12	–7.20	–7.20	–7.09	–7.14	–7.59
hexanoic acid	–2.08	–5.77	–7.86	–7.86	–7.71	–7.77	–8.23
p-hydroxybenzaldehyde	–2.28	–7.25	–9.53	–9.53	–8.95	–9.09	–11.63
water	–1.07	–2.07	–3.14	–3.14	–3.13	–3.12	–3.58
trimethylamine	–0.34	–2.34	–2.68	–2.68	–2.86	–2.74	–2.74
butylamine	–0.14	–4.43	–4.57	–4.57	–4.44	–4.48	–4.24
diethylamine	–0.21	–3.75	–3.96	–3.96	–3.73	–3.91	–3.78
pyridine	–0.95	–4.15	–5.10	–5.10	–5.24	–5.02	–4.88

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
aniline	–0.67	–6.05	–6.72	–6.72	–6.78	–6.84	–6.67
Solvent: ethyl ether							
n-octane	0.00	–5.01	–5.01	–5.01	–4.86	–4.88	–5.62
benzene	–0.49	–4.57	–5.06	–5.06	–5.20	–5.15	–4.21
toluene	–0.52	–4.96	–5.48	–5.48	–5.65	–5.61	–5.23
ethylbenzene	–0.49	–5.55	–6.05	–6.05	–6.04	–6.07	–5.45
o-xylene	–0.57	–5.34	–5.91	–5.91	–6.18	–6.11	–5.58
m-xylene	–0.55	–5.34	–5.89	–5.89	–6.11	–6.06	–5.56
naphthalene	–0.88	–7.28	–8.15	–8.15	–8.42	–8.33	–7.25
methanol	–0.95	–2.28	–3.23	–3.23	–3.19	–3.18	–3.61
ethanol	–0.83	–3.24	–4.07	–4.07	–4.15	–4.09	–4.41
1,2-ethanediol	–1.42	–4.84	–6.27	–6.27	–6.35	–6.47	–6.20
1-propanol	–0.80	–3.92	–4.72	–4.72	–4.71	–4.70	–4.90
2-propanol	–0.78	–3.77	–4.55	–4.55	–4.38	–4.46	–4.44
1-butanol	–0.80	–4.59	–5.39	–5.39	–5.26	–5.31	–5.69
2-methyl-2-propanol	–0.70	–4.01	–4.72	–4.72	–4.74	–4.71	–4.80
cyclopentanol	–0.71	–5.51	–6.22	–6.22	–6.05	–6.09	–6.50
1-pentanol	–0.80	–5.24	–6.04	–6.04	–5.87	–5.93	–6.11
phenol	–1.04	–6.34	–7.38	–7.38	–7.34	–7.28	–8.75
1-hexanol	–0.84	–5.79	–6.63	–6.63	–6.45	–6.56	–6.82
m-cresol	–1.07	–6.71	–7.78	–7.78	–7.79	–7.73	–7.95
1-heptanol	–0.83	–6.45	–7.28	–7.28	–7.07	–7.20	–7.51
1-octanol	–0.79	–7.19	–7.98	–7.98	–7.74	–7.83	–7.25
1,4-dioxane	–1.89	–3.10	–4.99	–4.99	–5.04	–5.00	–4.67
anisole	–1.21	–4.84	–6.06	–6.06	–6.06	–5.92	–5.71
ethanal	–1.73	–1.61	–3.34	–3.34	–3.26	–3.32	–2.85
propanal	–1.53	–2.28	–3.80	–3.80	–3.88	–3.86	–3.85
benzaldehyde	–1.83	–5.46	–7.28	–7.28	–7.02	–7.09	–6.08
butanone	–1.53	–3.02	–4.54	–4.54	–4.70	–4.62	–4.09

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
methyl phenyl ketone	–1.92	–6.15	–8.06	–8.06	–7.84	–7.85	–6.79
ethanoic acid	–2.55	–3.15	–5.71	–5.71	–5.73	–5.71	–6.26
propanoic acid	–2.27	–3.82	–6.08	–6.08	–6.11	–6.09	–6.75
butanoic acid	–2.21	–4.45	–6.66	–6.66	–6.55	–6.60	–7.32
pentanoic acid	–2.18	–5.10	–7.27	–7.27	–7.19	–7.24	–7.87
hexanoic acid	–2.17	–5.75	–7.92	–7.92	–7.80	–7.86	–8.85
2-propen-1-ol	–0.83	–3.80	–4.62	–4.62	–4.17	–4.36	–4.87
2-methoxyethanol	–1.45	–3.90	–5.35	–5.35	–5.16	–5.29	–5.12
m-hydroxybenzaldehyde	–2.25	–7.23	–9.48	–9.48	–8.97	–9.10	–11.36
p-hydroxybenzaldehyde	–2.38	–7.21	–9.59	–9.59	–9.12	–9.22	–12.07
water	–1.11	–2.08	–3.19	–3.19	–3.21	–3.19	–3.85
methylamine	–0.18	–2.31	–2.49	–2.49	–2.44	–2.36	–2.32
ethylamine	–0.17	–3.07	–3.24	–3.24	–3.14	–3.15	–2.89
dimethylamine	–0.25	–2.37	–2.62	–2.62	–2.62	–2.60	–2.63
propylamine	–0.15	–3.75	–3.90	–3.90	–3.80	–3.82	–3.65
trimethylamine	–0.35	–2.33	–2.68	–2.68	–2.87	–2.74	–2.78
butylamine	–0.14	–4.41	–4.55	–4.55	–4.43	–4.46	–4.44
diethylamine	–0.22	–3.74	–3.95	–3.95	–3.72	–3.89	–3.83
piperidine	–0.19	–4.81	–5.01	–5.01	–5.06	–5.08	–4.82
dipropylamine	–0.17	–5.08	–5.25	–5.25	–4.94	–5.21	–4.96
pyridine	–0.99	–4.12	–5.12	–5.12	–5.33	–5.06	–4.81
aniline	–0.69	–6.01	–6.71	–6.71	–6.86	–6.88	–6.51
ethanonitrile	–1.40	–1.32	–2.72	–2.72	–2.87	–3.31	–3.59
benzonitrile	–1.26	–5.15	–6.42	–6.42	–5.90	–6.29	–6.36
nitrobenzene	–4.09	–3.12	–7.21	–7.21	–6.98	–7.20	–6.85
2-methyl-1-nitrobenzene	–3.81	–3.60	–7.41	–7.41	–7.34	–7.34	–7.21
ethanamide	–1.63	–3.34	–4.97	–4.97	–4.96	–4.53	–6.16
ammonia	–0.14	–2.23	–2.37	–2.37	–2.42	–2.15	–1.41
hydrazine	–0.16	–6.30	–6.46	–6.46	–6.34	–6.37	–6.11

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
hydrogen sulfide	–0.08	–0.64	–0.72	–0.63	–0.89	–0.72	–0.60
chlorobenzene	–0.78	–5.16	–5.94	–6.02	–5.84	–5.86	–5.42
p-dichlorobenzene	–0.76	–5.75	–6.51	–6.62	–6.17	–6.46	–6.18
bromobenzene	–0.70	–5.88	–6.59	–6.56	–6.66	–6.52	–5.99
iodomethane	–0.41	–2.40	–2.80	–2.59	–2.56	–3.37	–3.51
iodobenzene	–0.66	–6.57	–7.23	–7.34	–7.46	–6.74	–6.64
Solvent: anisole							
n-octane	0.00	–4.79	–4.80	–4.80	–4.59	–4.64	–4.62
toluene	–0.52	–4.90	–5.42	–5.42	–5.51	–5.51	–4.95
ethanol	–0.83	–2.81	–3.64	–3.64	–3.68	–3.66	–3.59
1,4-dioxane	–1.88	–3.03	–4.91	–4.91	–4.83	–4.92	–5.06
butanone	–1.53	–2.84	–4.37	–4.37	–4.45	–4.44	–4.43
Solvent: ethoxybenzene							
n-octane	0.00	–4.84	–4.84	–4.84	–4.63	–4.68	–4.75
toluene	–0.52	–4.93	–5.45	–5.45	–5.52	–5.53	–4.99
ethanol	–0.83	–2.91	–3.74	–3.74	–3.78	–3.75	–3.45
1,4-dioxane	–1.88	–3.05	–4.92	–4.92	–4.85	–4.93	–4.87
butanone	–1.52	–2.88	–4.40	–4.40	–4.48	–4.46	–4.28
Solvent: phenylether							
n-octane	0.00	–5.79	–5.79	–5.79	–5.91	–5.79	–4.38
toluene	–0.50	–5.55	–6.04	–6.04	–6.27	–6.20	–4.86
ethanol	–0.79	–2.96	–3.75	–3.75	–3.89	–3.82	–3.22
1,4-dioxane	–1.80	–3.62	–5.42	–5.42	–5.43	–5.51	–4.83
butanone	–1.45	–3.37	–4.82	–4.82	–5.04	–4.96	–4.08
Solvent: triethylamine							
n-octane	0.00	–4.46	–4.46	–4.46	–4.42	–4.39	–5.62
toluene	–0.38	–4.92	–5.30	–5.30	–4.57	–4.95	–4.98
ethanol	–0.61	–4.11	–4.72	–4.72	–4.61	–4.67	–3.87
1,4-dioxane	–1.39	–2.74	–4.14	–4.14	–4.05	–4.29	–4.41

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
butanone	–1.08	–2.85	–3.93	–3.93	–3.77	–3.66	–3.86
Solvent: aniline							
n-octane	0.00	–4.26	–4.26	–4.26	–3.82	–3.98	–3.48
toluene	–0.59	–4.48	–5.07	–5.07	–5.06	–5.12	–4.57
ethanol	–0.94	–3.73	–4.68	–4.68	–4.71	–4.69	–4.45
1,4-dioxane	–2.14	–2.89	–5.03	–5.03	–4.93	–5.01	–5.65
butanone	–1.78	–2.83	–4.61	–4.61	–4.69	–4.70	–4.87
ethanoic acid	–2.93	–3.19	–6.12	–6.12	–6.09	–6.11	–6.30
propanoic acid	–2.60	–3.81	–6.40	–6.40	–6.35	–6.38	–6.20
Solvent: pyridine							
n-octane	0.00	–4.61	–4.61	–4.61	–4.29	–4.40	–4.50
toluene	–0.65	–4.94	–5.59	–5.59	–5.89	–5.82	–5.10
ethanol	–1.03	–3.40	–4.43	–4.43	–4.52	–4.46	–5.08
1,4-dioxane	–2.33	–2.89	–5.23	–5.23	–5.31	–5.21	–5.14
butanone	–1.98	–2.83	–4.81	–4.81	–5.05	–4.98	–4.61
Solvent:2-methyl pyridine							
n-octane	0.00	–4.63	–4.63	–4.63	–4.33	–4.43	–4.73
toluene	–0.63	–4.98	–5.61	–5.61	–5.81	–5.78	–5.06
ethanol	–1.00	–3.58	–4.58	–4.58	–4.65	–4.60	–5.01
1,4-dioxane	–2.27	–2.89	–5.16	–5.16	–5.25	–5.16	–5.01
butanone	–1.91	–2.86	–4.77	–4.77	–4.98	–4.89	–4.52
Solvent: dimethylpyridine							
n-octane	0.00	–4.63	–4.64	–4.64	–4.38	–4.46	–4.88
toluene	–0.60	–5.02	–5.62	–5.62	–5.67	–5.71	–5.03
ethanol	–0.95	–3.72	–4.67	–4.67	–4.72	–4.68	–4.87
1,4-dioxane	–2.15	–2.89	–5.04	–5.04	–5.11	–5.07	–4.90
butanone	–1.80	–2.89	–4.68	–4.68	–4.83	–4.74	–4.34
Solvent: acetonitrile							
n-octane	0.00	–4.05	–4.05	–4.05	–3.67	–3.81	–3.57

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
toluene	–0.70	–4.20	–4.89	–4.89	–5.68	–5.37	–4.68
ethanol	–1.09	–2.80	–3.90	–3.90	–4.11	–3.97	–4.43
1,4-dioxane	–2.48	–2.61	–5.09	–5.09	–5.29	–5.00	–5.33
butanone	–2.14	–2.50	–4.64	–4.64	–5.07	–5.00	–4.73
Solvent: benzonitrile							
n-octane	0.00	–5.14	–5.15	–5.15	–4.96	–5.00	–4.34
toluene	–0.69	–5.17	–5.85	–5.85	–6.54	–6.28	–4.95
ethanol	–1.08	–3.07	–4.14	–4.14	–4.36	–4.23	–4.05
1,4-dioxane	–2.44	–3.23	–5.67	–5.67	–5.85	–5.65	–5.14
butanone	–2.10	–3.06	–5.16	–5.16	–5.59	–5.50	–4.58
Solvent: nitromethane							
n-octane	0.00	–3.68	–3.68	–3.68	–3.20	–3.39	–3.15
toluene	–0.69	–4.00	–4.69	–4.69	–5.39	–5.13	–4.52
ethanol	–1.09	–2.60	–3.69	–3.69	–3.85	–3.74	–4.16
1,4-dioxane	–2.48	–2.40	–4.88	–4.88	–5.00	–4.77	–5.46
butanone	–2.14	–2.27	–4.41	–4.41	–4.76	–4.74	–4.72
Solvent: nitroethane							
n-octane	0.00	–4.10	–4.10	–4.10	–3.70	–3.85	–3.89
toluene	–0.69	–4.33	–5.02	–5.02	–5.72	–5.45	–4.88
ethanol	–1.08	–2.70	–3.79	–3.79	–3.96	–3.84	–3.98
1,4-dioxane	–2.45	–2.61	–5.07	–5.07	–5.21	–4.98	–5.28
butanone	–2.12	–2.48	–4.59	–4.59	–4.96	–4.91	–4.73
Solvent: nitrobenzene							
methanol	–1.24	–1.65	–2.89	–2.89	–2.90	–2.86	–2.93
phenol	–1.37	–5.77	–7.14	–7.14	–7.56	–7.30	–7.86
o-cresol	–1.40	–6.04	–7.45	–7.45	–7.94	–7.67	–8.16
m-cresol	–1.41	–6.05	–7.46	–7.46	–7.92	–7.69	–7.29
p-cresol	–1.38	–6.06	–7.43	–7.43	–7.84	–7.65	–8.13
ethanoic acid	–3.44	–2.43	–5.87	–5.87	–6.04	–6.03	–4.78

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
propanoic acid	–3.05	–3.04	–6.09	–6.09	–6.25	–6.25	–5.38
butanoic acid	–2.98	–3.61	–6.59	–6.59	–6.52	–6.64	–5.84
pentanoic acid	–2.94	–4.20	–7.14	–7.14	–7.08	–7.21	–6.47
hexanoic acid	–2.93	–4.80	–7.73	–7.73	–7.59	–7.75	–7.26
aniline	–0.92	–5.62	–6.54	–6.54	–7.15	–7.02	–7.15
p-bromophenol	–1.65	–7.14	–8.79	–8.73	–9.15	–8.83	–9.76
Solvent: *o*-nitrotoluene							
phenol	–1.36	–5.76	–7.12	–7.12	–7.54	–7.28	–7.79
ethanoic acid	–3.39	–2.42	–5.82	–5.82	–6.00	–5.98	–4.68
propanoic acid	–3.01	–3.04	–6.06	–6.06	–6.22	–6.21	–5.30
butanoic acid	–2.94	–3.62	–6.56	–6.56	–6.50	–6.61	–5.76
p-bromophenol	–1.63	–7.13	–8.76	–8.70	–9.13	–8.80	–9.57
Solvent: dimethylformamide							
n-octane	0.00	–3.64	–3.64	–3.64	–3.25	–3.41	–3.77
toluene	–0.69	–4.38	–5.08	–5.08	–5.37	–5.32	–4.88
ethanol	–1.09	–3.64	–4.73	–4.73	–4.82	–4.75	–5.23
1,4-dioxane	–2.48	–2.29	–4.77	–4.77	–4.96	–4.76	–5.03
butanone	–2.14	–2.36	–4.51	–4.51	–4.78	–4.66	–4.56
Solvent: dimethylacetamide							
n-octane	0.00	–3.73	–3.74	–3.74	–3.42	–3.54	–3.94
toluene	–0.70	–4.48	–5.18	–5.18	–5.47	–5.42	–4.94
ethanol	–1.10	–3.79	–4.88	–4.88	–5.00	–4.92	–5.40
1,4-dioxane	–2.48	–2.35	–4.83	–4.83	–5.06	–4.84	–5.01
butanone	–2.15	–2.43	–4.58	–4.58	–4.88	–4.74	–4.52
Solvent: fluoroctane							
methyl ethanoate	–2.35	–1.42	–3.77	–3.77	–4.00	–3.84	–3.59
methyl propanoate	–2.12	–2.05	–4.17	–4.17	–4.40	–4.25	–4.09
ethyl ethanoate	–2.30	–2.27	–4.57	–4.57	–4.74	–4.62	–4.16
propyl ethanoate	–2.25	–2.91	–5.16	–5.16	–5.28	–5.22	–4.65

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
methyl pentanoate	–2.04	–3.27	–5.31	–5.31	–5.45	–5.36	–5.33
butyl ethanoate	–2.22	–3.53	–5.75	–5.75	–5.86	–5.81	–5.22
Solvent: methylenechloride							
n-octane	0.00	–5.24	–5.25	–5.25	–5.09	–5.11	–5.18
toluene	–0.62	–4.83	–5.46	–5.46	–6.28	–5.94	–5.53
ethanol	–0.98	–2.60	–3.59	–3.59	–3.85	–3.69	–3.82
phenol	–1.23	–5.53	–6.77	–6.77	–7.45	–7.07	–7.50
p-cresol	–1.24	–5.95	–7.18	–7.18	–7.87	–7.54	–7.71
1,4-dioxane	–2.23	–3.36	–5.59	–5.59	–5.73	–5.55	–4.82
water	–1.31	–0.47	–1.78	–1.78	–2.04	–1.91	–2.63
thiophenol	–1.02	–5.81	–6.83	–6.85	–7.29	–7.09	–7.11
p-bromophenol	–1.48	–7.01	–8.49	–8.43	–9.09	–8.66	–9.09
Solvent: chloroform							
n-octane	0.00	–5.49	–5.49	–5.49	–5.37	–5.37	–5.25
cyclohexane	0.00	–4.42	–4.42	–4.42	–4.64	–4.44	–4.45
benzene	–0.51	–4.51	–5.02	–5.02	–5.51	–5.29	–4.64
toluene	–0.54	–4.95	–5.49	–5.49	–6.01	–5.80	–5.48
ethylbenzene	–0.51	–5.61	–6.12	–6.12	–6.46	–6.32	–5.84
o-xylene	–0.59	–5.39	–5.97	–5.97	–6.60	–6.35	–6.23
m-xylene	–0.57	–5.39	–5.96	–5.96	–6.52	–6.31	–5.86
naphthalene	–0.91	–7.19	–8.10	–8.10	–8.93	–8.56	–7.89
methanol	–0.98	–1.74	–2.72	–2.72	–2.78	–2.73	–3.32
ethanol	–0.86	–2.77	–3.63	–3.63	–3.82	–3.72	–3.94
1,2-ethanediol	–1.47	–3.75	–5.22	–5.22	–5.44	–5.44	–5.98
1-propanol	–0.83	–3.52	–4.35	–4.35	–4.44	–4.38	–4.41
2-propanol	–0.81	–3.38	–4.19	–4.19	–4.11	–4.15	–4.28
1-butanol	–0.83	–4.26	–5.09	–5.09	–5.06	–5.07	–5.28
2-methyl-2-propanol	–0.73	–3.66	–4.39	–4.39	–4.51	–4.44	–4.48
1-pentanol	–0.82	–4.98	–5.80	–5.80	–5.73	–5.75	–5.90

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
phenol	–1.08	–5.71	–6.79	–6.79	–7.18	–6.94	–7.14
1-hexanol	–0.86	–5.66	–6.53	–6.53	–6.43	–6.51	–6.67
o-cresol	–1.09	–6.13	–7.22	–7.22	–7.68	–7.42	–7.55
m-cresol	–1.11	–6.14	–7.25	–7.25	–7.68	–7.45	–6.70
p-cresol	–1.08	–6.15	–7.23	–7.23	–7.63	–7.43	–7.59
1-heptanol	–0.86	–6.38	–7.25	–7.25	–7.11	–7.21	–7.53
1,4-dioxane	–1.95	–3.54	–5.50	–5.50	–5.51	–5.48	–6.21
diethyl ether	–0.83	–2.97	–3.80	–3.80	–3.89	–3.82	–4.32
anisole	–1.26	–4.94	–6.20	–6.20	–6.53	–6.26	–6.24
tetrahydropyran	–0.92	–4.11	–5.03	–5.03	–5.17	–5.06	–5.84
isopropyl ether	–0.81	–4.01	–4.82	–4.82	–4.56	–4.68	–3.78
ethyl phenyl ether	–1.14	–5.86	–7.00	–7.00	–7.28	–7.06	–7.16
formaldehyde	–1.92	–0.36	–2.28	–2.28	–2.16	–2.31	0.12
ethanal	–1.80	–1.74	–3.54	–3.54	–3.57	–3.72	–3.65
benzaldehyde	–1.90	–5.49	–7.38	–7.38	–7.54	–7.54	–7.09
propanone	–1.79	–2.57	–4.36	–4.36	–4.54	–4.58	–4.42
butanone	–1.59	–3.28	–4.87	–4.87	–5.15	–5.14	–5.43
methyl phenyl ketone	–1.99	–6.25	–8.24	–8.24	–8.43	–8.36	–7.81
ethanoic acid	–2.65	–2.33	–4.98	–4.98	–5.19	–5.13	–4.74
propanoic acid	–2.35	–3.06	–5.41	–5.41	–5.63	–5.56	–5.37
butanoic acid	–2.29	–3.76	–6.05	–6.05	–6.12	–6.13	–5.99
pentanoic acid	–2.26	–4.47	–6.73	–6.73	–6.83	–6.83	–6.61
hexanoic acid	–2.25	–5.19	–7.45	–7.45	–7.50	–7.51	–7.51
methyl ethanoate	–2.52	–1.68	–4.21	–4.21	–4.42	–4.28	–4.90
methyl propanoate	–2.27	–2.41	–4.68	–4.68	–4.89	–4.76	–5.48
ethyl ethanoate	–2.46	–2.64	–5.11	–5.11	–5.24	–5.15	–5.58
propyl ethanoate	–2.41	–3.37	–5.79	–5.79	–5.85	–5.82	–6.35
methyl pentanoate	–2.19	–3.82	–6.01	–6.01	–6.07	–6.02	–6.68
butyl ethanoate	–2.38	–4.09	–6.47	–6.47	–6.50	–6.50	–6.71

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
methyl hexanoate	–2.19	–4.54	–6.72	–6.72	–6.74	–6.71	–7.24
pentyl ethanoate	–2.38	–4.80	–7.18	–7.18	–7.18	–7.19	–7.36
methyl benzoate	–2.52	–5.32	–7.83	–7.83	–7.71	–7.62	–7.81
2-propen-1-ol	–0.86	–3.25	–4.11	–4.11	–3.84	–3.95	–4.34
p-hydroxybenzaldehyde	–2.47	–6.65	–9.12	–9.12	–9.15	–9.18	–10.30
water	–1.15	–0.60	–1.75	–1.75	–1.95	–1.84	–2.05
methylamine	–0.19	–2.40	–2.59	–2.59	–2.56	–2.49	–3.17
ethylamine	–0.17	–3.25	–3.42	–3.42	–3.37	–3.37	–4.02
dimethylamine	–0.26	–2.92	–3.18	–3.18	–3.06	–3.11	–3.69
propylamine	–0.15	–4.00	–4.16	–4.16	–4.10	–4.12	–4.73
trimethylamine	–0.37	–3.24	–3.60	–3.60	–3.57	–3.54	–3.90
butylamine	–0.15	–4.72	–4.87	–4.87	–4.80	–4.83	–5.35
diethylamine	–0.23	–4.41	–4.63	–4.63	–4.34	–4.56	–5.23
piperidine	–0.20	–5.62	–5.82	–5.82	–5.81	–5.88	–6.37
pyridine	–1.03	–4.61	–5.64	–5.64	–6.00	–5.62	–6.45
2-methylpyrazine	–1.44	–5.28	–6.72	–6.72	–7.14	–6.56	–6.99
aniline	–0.72	–5.78	–6.50	–6.50	–7.05	–6.90	–7.34
2-methylpyridine	–1.10	–5.17	–6.26	–6.26	–6.79	–6.32	–6.98
3-methylpyridine	–1.01	–5.05	–6.06	–6.06	–6.47	–6.12	–7.35
4-methylpyridine	–1.04	–5.05	–6.09	–6.09	–6.53	–6.17	–7.50
2-ethylpyrazine	–1.34	–5.95	–7.29	–7.29	–7.55	–7.09	–7.72
2,6-dimethylpyridine	–1.18	–5.73	–6.91	–6.91	–7.58	–7.04	–7.74
ethanonitrile	–1.46	–1.84	–3.30	–3.30	–3.50	–3.88	–4.44
benzonitrile	–1.31	–5.60	–6.92	–6.92	–6.75	–6.91	–7.22
nitrobenzene	–4.25	–3.70	–7.95	–7.95	–7.59	–7.94	–7.78
2-methyl-1-nitrobenzene	–3.97	–4.21	–8.17	–8.17	–8.00	–8.10	–8.30
ethanamide	–1.69	–3.31	–5.00	–5.00	–5.15	–4.77	–7.05
1,1-dimethyl-3-phenylurea	–2.88	–8.19	–11.07	–11.07	–11.06	–11.69	–13.64
9-methyladenine	–4.29	–10.46	–14.75	–14.75	–15.21	–14.66	–12.51

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
1-methylthymine	–4.71	–6.36	–11.07	–11.07	–10.48	–11.21	–9.71
morpholine	–1.15	–5.25	–6.41	–6.41	–6.41	–6.48	–6.72
ammonia	–0.14	–1.83	–1.97	–1.97	–2.19	–1.85	–2.41
hydrazine	–0.16	–6.23	–6.40	–6.40	–6.48	–6.44	–7.46
thiophenol	–0.88	–6.06	–6.94	–6.98	–7.09	–7.04	–7.61
thiophene	–1.84	–4.30	–6.14	–5.56	–6.05	–5.53	–5.83
diethyl sulfide	–0.11	–4.32	–4.42	–4.58	–4.48	–4.60	–6.40
hydrogen sulfide	–0.09	–1.65	–1.74	–1.68	–1.52	–1.53	–0.51
thioanisole	–0.79	–6.46	–7.25	–7.44	–7.70	–7.72	–5.98
fluorobenzene	–1.51	–3.75	–5.26	–5.29	–5.03	–5.01	–4.25
chlorobenzene	–0.81	–5.29	–6.10	–6.17	–6.24	–6.14	–5.45
p-dichlorobenzene	–0.78	–6.05	–6.84	–6.95	–6.63	–6.86	–6.32
bromobenzene	–0.73	–6.08	–6.81	–6.78	–7.11	–6.86	–6.07
iodobenzene	–0.68	–6.85	–7.53	–7.64	–7.98	–7.12	–6.60
difluorodichloromethane	–0.34	–1.50	–1.84	–1.69	–1.89	–2.44	–1.55
fluorotrichloromethane	–0.19	–3.07	–3.26	–3.01	–3.32	–3.78	–2.62
2,2,2-trifluoroethanol	–3.19	–1.06	–4.25	–4.33	–4.14	–3.84	–3.03
p-bromophenol	–1.29	–7.25	–8.54	–8.48	–8.87	–8.59	–8.59
Solvent: carbon tetrachloride							
n-octane	0.00	–5.95	–5.95	–5.95	–5.94	–5.88	–5.25
2-methylpropene	–0.11	–2.42	–2.53	–2.53	–2.42	–2.46	–2.63
1-butene	–0.07	–2.63	–2.70	–2.70	–2.44	–2.55	–2.48
E-2-pentene	–0.08	–3.63	–3.71	–3.71	–3.54	–3.60	–3.46
benzene	–0.34	–4.90	–5.24	–5.24	–5.13	–5.19	–4.50
toluene	–0.36	–5.38	–5.74	–5.74	–5.67	–5.72	–5.12
ethylbenzene	–0.34	–6.09	–6.43	–6.43	–6.25	–6.34	–5.67
o-xylene	–0.39	–5.86	–6.25	–6.25	–6.26	–6.28	–6.07
m-xylene	–0.38	–5.86	–6.24	–6.24	–6.21	–6.25	–5.71
naphthalene	–0.60	–7.76	–8.36	–8.36	–8.20	–8.28	–7.55

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
methanol	–0.66	–1.35	–2.02	–2.02	–1.91	–1.99	–2.25
ethanol	–0.58	–2.44	–3.02	–3.02	–3.04	–3.04	–2.96
1-propanol	–0.56	–3.23	–3.80	–3.80	–3.76	–3.79	–3.64
2-propanol	–0.55	–3.10	–3.65	–3.65	–3.50	–3.60	–3.15
1-butanol	–0.56	–4.03	–4.59	–4.59	–4.49	–4.55	–4.20
2-methyl-2-propanol	–0.49	–3.43	–3.92	–3.92	–3.93	–3.94	–3.40
1-pentanol	–0.56	–4.79	–5.35	–5.35	–5.25	–5.31	–4.73
phenol	–0.72	–5.61	–6.34	–6.34	–6.10	–6.16	–6.14
1-hexanol	–0.59	–5.55	–6.14	–6.14	–6.02	–6.12	–5.04
o-cresol	–0.73	–6.08	–6.81	–6.81	–6.63	–6.68	–6.51
p-cresol	–0.73	–6.11	–6.83	–6.83	–6.61	–6.69	–6.32
1-heptanol	–0.59	–6.32	–6.90	–6.90	–6.78	–6.88	–6.49
1,4-dioxane	–1.32	–3.71	–5.03	–5.03	–4.79	–5.07	–4.97
anisole	–0.83	–5.28	–6.11	–6.11	–5.79	–5.92	–5.49
benzaldehyde	–1.23	–5.76	–6.99	–6.99	–6.48	–6.73	–6.11
propanone	–1.14	–2.62	–3.76	–3.76	–3.67	–3.75	–3.35
butanone	–1.01	–3.38	–4.39	–4.39	–4.40	–4.42	–4.09
cyclopentanone	–1.01	–4.59	–5.60	–5.60	–5.48	–5.53	–5.26
2-pentanone	–1.01	–4.11	–5.12	–5.12	–5.05	–5.11	–4.81
2-hexanone	–0.93	–4.89	–5.82	–5.82	–5.79	–5.81	–5.47
2-heptanone	–0.99	–5.64	–6.63	–6.63	–6.58	–6.62	–6.12
methyl phenyl ketone	–1.28	–6.57	–7.85	–7.85	–7.38	–7.57	–7.10
ethanoic acid	–1.75	–2.23	–3.98	–3.98	–3.95	–3.95	–3.64
propanoic acid	–1.55	–3.01	–4.56	–4.56	–4.56	–4.54	–4.09
butanoic acid	–1.51	–3.75	–5.27	–5.27	–5.19	–5.21	–4.81
hexanoic acid	–1.49	–5.28	–6.77	–6.77	–6.72	–6.72	–6.99
methyl ethanoate	–1.67	–1.99	–3.65	–3.65	–3.57	–3.61	–3.82
methyl propanoate	–1.50	–2.76	–4.27	–4.27	–4.19	–4.22	–4.43
ethyl ethanoate	–1.62	–3.00	–4.62	–4.62	–4.50	–4.56	–4.40

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
propyl ethanoate	–1.59	–3.78	–5.37	–5.37	–5.22	–5.31	–5.03
methyl pentanoate	–1.45	–4.27	–5.72	–5.72	–5.59	–5.65	–5.71
butyl ethanoate	–1.57	–4.54	–6.11	–6.11	–5.96	–6.05	–5.59
methyl hexanoate	–1.45	–5.04	–6.48	–6.48	–6.34	–6.40	–6.39
pentyl ethanoate	–1.57	–5.31	–6.87	–6.87	–6.72	–6.81	–6.35
methyl benzoate	–1.65	–5.88	–7.53	–7.53	–6.82	–7.09	–7.19
p-hydroxybenzaldehyde	–1.62	–6.44	–8.06	–8.06	–7.41	–7.68	–8.16
water	–0.78	0.32	–0.46	–0.46	–0.45	–0.44	–0.85
methylamine	–0.13	–2.06	–2.19	–2.19	–2.09	–2.11	–2.53
ethylamine	–0.12	–2.94	–3.06	–3.06	–2.94	–3.01	–2.77
dimethylamine	–0.18	–2.61	–2.79	–2.79	–2.60	–2.74	–2.75
propylamine	–0.11	–3.74	–3.84	–3.84	–3.74	–3.81	–3.59
trimethylamine	–0.25	–3.01	–3.27	–3.27	–3.18	–3.25	–3.09
butylamine	–0.10	–4.50	–4.61	–4.61	–4.51	–4.57	–4.34
diethylamine	–0.15	–4.17	–4.33	–4.33	–4.04	–4.28	–4.12
pyridine	–0.68	–4.71	–5.39	–5.39	–5.27	–5.22	–5.01
aniline	–0.48	–5.89	–6.37	–6.37	–6.29	–6.40	–6.10
benzonitrile	–0.84	–5.85	–6.69	–6.69	–6.08	–6.46	–6.28
1-nitropropane	–3.05	–2.10	–5.16	–5.16	–5.42	–5.29	–4.49
nitrobenzene	–2.76	–4.47	–7.23	–7.23	–6.66	–7.01	–6.92
2-methyl-1-nitrobenzene	–2.56	–4.99	–7.55	–7.55	–7.12	–7.31	–7.49
ammonia	–0.10	–1.49	–1.59	–1.59	–1.70	–1.49	–1.06
thioanisole	–0.52	–6.77	–7.30	–7.45	–7.18	–7.40	–5.66
fluorobenzene	–0.97	–4.12	–5.10	–5.12	–4.55	–4.78	–3.64
chlorobenzene	–0.53	–5.68	–6.20	–6.22	–5.89	–6.04	–5.21
p-dichlorobenzene	–0.52	–6.45	–6.97	–6.98	–6.46	–6.83	–6.28
bromobenzene	–0.48	–6.48	–6.96	–6.91	–6.76	–6.79	–5.85
iodobenzene	–0.45	–7.26	–7.71	–7.82	–7.64	–7.11	–6.50
p-bromophenol	–0.86	–7.17	–8.04	–7.96	–7.79	–7.81	–7.86

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			Expt
				MNDO	AM1	PM3	
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
Solvent: dichloroethane							
methanol	–1.14	–1.60	–2.74	–2.74	–2.82	–2.75	–2.53
ethanol	–1.00	–2.54	–3.54	–3.54	–3.76	–3.63	–2.83
1-propanol	–0.97	–3.19	–4.16	–4.16	–4.25	–4.19	–3.85
1-butanol	–0.96	–3.85	–4.81	–4.81	–4.73	–4.75	–4.92
1-pentanol	–0.96	–4.47	–5.43	–5.43	–5.29	–5.34	–5.45
phenol	–1.26	–5.43	–6.69	–6.69	–7.27	–6.94	–7.48
1-hexanol	–1.01	–5.06	–6.06	–6.06	–5.88	–6.00	–6.02
o-cresol	–1.28	–5.75	–7.04	–7.04	–7.69	–7.34	–7.73
m-cresol	–1.29	–5.76	–7.06	–7.06	–7.68	–7.37	–6.91
p-cresol	–1.26	–5.78	–7.04	–7.04	–7.62	–7.34	–7.75
1-heptanol	–1.00	–5.68	–6.69	–6.69	–6.45	–6.60	–6.79
benzaldehyde	–2.27	–5.03	–7.30	–7.30	–7.69	–7.59	–7.23
methyl phenyl ketone	–2.40	–5.71	–8.10	–8.10	–8.53	–8.36	–7.83
ethanoic acid	–3.13	–2.20	–5.33	–5.33	–5.59	–5.53	–4.89
propanoic acid	–2.78	–2.84	–5.62	–5.62	–5.87	–5.82	–5.12
butanoic acid	–2.71	–3.44	–6.15	–6.15	–6.21	–6.26	–5.83
pentanoic acid	–2.67	–4.07	–6.74	–6.74	–6.81	–6.86	–6.47
hexanoic acid	–2.67	–4.69	–7.36	–7.36	–7.37	–7.45	–7.33
methyl ethanoate	–2.98	–1.31	–4.29	–4.29	–4.62	–4.40	–4.55
methyl propanoate	–2.68	–1.95	–4.63	–4.63	–4.93	–4.74	–4.87
ethyl ethanoate	–2.91	–2.18	–5.09	–5.09	–5.31	–5.16	–4.93
propyl ethanoate	–2.85	–2.82	–5.67	–5.67	–5.78	–5.73	–5.40
methyl pentanoate	–2.58	–3.17	–5.76	–5.76	–5.86	–5.78	–5.97
butyl ethanoate	–2.82	–3.44	–6.26	–6.26	–6.31	–6.30	–5.93
methyl hexanoate	–2.58	–3.80	–6.38	–6.38	–6.40	–6.36	–6.57
pentyl ethanoate	–2.80	–4.07	–6.87	–6.87	–6.88	–6.89	–6.64
m-hydroxybenzaldehyde	–2.76	–6.28	–9.04	–9.04	–9.21	–9.18	–10.11
p-hydroxybenzaldehyde	–2.93	–6.25	–9.19	–9.19	–9.41	–9.37	–10.70

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
ethylamine	–0.20	–2.85	–3.05	–3.05	–2.96	–2.95	–3.19
propylamine	–0.18	–3.52	–3.69	–3.69	–3.58	–3.60	–4.04
butylamine	–0.17	–4.14	–4.32	–4.32	–4.17	–4.21	–4.49
diethylamine	–0.26	–3.74	–4.00	–4.00	–3.65	–3.87	–4.00
pyridine	–1.22	–4.13	–5.35	–5.35	–5.93	–5.39	–5.53
aniline	–0.84	–5.41	–6.25	–6.25	–7.00	–6.77	–7.39
p-bromophenol	–1.51	–6.84	–8.35	–8.29	–8.85	–8.47	–9.10
Solvent: tetrachloroethene							
phenol	–0.73	–5.32	–6.05	–6.05	–5.78	–5.86	–6.10
propanone	–1.16	–2.33	–3.49	–3.49	–3.38	–3.47	–3.09
methyl ethanoate	–1.69	–1.64	–3.33	–3.33	–3.22	–3.28	–3.63
methyl propanoate	–1.53	–2.36	–3.88	–3.88	–3.79	–3.84	–4.39
ethyl ethanoate	–1.65	–2.60	–4.25	–4.25	–4.10	–4.18	–4.22
propyl ethanoate	–1.62	–3.31	–4.93	–4.93	–4.76	–4.86	–4.80
methyl pentanoate	–1.47	–3.74	–5.21	–5.21	–5.05	–5.13	–5.41
butyl ethanoate	–1.60	–4.02	–5.62	–5.62	–5.43	–5.54	–5.35
Solvent: chlorohexane							
propanone	–1.92	–2.07	–3.99	–3.99	–4.26	–4.25	–3.45
butanone	–1.72	–2.69	–4.40	–4.40	–4.80	–4.73	–4.10
2-pentanone	–1.70	–3.28	–4.98	–4.98	–5.25	–5.23	–4.84
2-hexanone	–1.57	–3.92	–5.49	–5.49	–5.80	–5.74	–5.42
3,3-dimethylbutanone	–1.60	–3.07	–4.67	–4.67	–5.02	–4.92	–4.98
methyl ethanoate	–2.70	–1.39	–4.08	–4.08	–4.42	–4.21	–3.66
methyl propanoate	–2.43	–2.02	–4.45	–4.45	–4.78	–4.58	–4.20
ethyl ethanoate	–2.63	–2.25	–4.88	–4.88	–5.15	–4.98	–4.25
propyl ethanoate	–2.58	–2.89	–5.46	–5.46	–5.66	–5.56	–4.84
methyl pentanoate	–2.34	–3.24	–5.58	–5.58	–5.79	–5.66	–5.41
butyl ethanoate	–2.55	–3.51	–6.05	–6.05	–6.22	–6.15	–5.37

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
Solvent: bromoform							
methanol	–0.95	–1.65	–2.60	–2.60	–2.50	–2.55	–2.79
ethanol	–0.83	–2.67	–3.50	–3.50	–3.51	–3.51	–3.24
1-propanol	–0.81	–3.37	–4.18	–4.18	–4.05	–4.12	–4.03
1-butanol	–0.80	–4.07	–4.88	–4.88	–4.60	–4.74	–4.72
1-pentanol	–0.80	–4.75	–5.54	–5.54	–5.21	–5.37	–5.34
phenol	–1.04	–5.75	–6.79	–6.79	–6.72	–6.70	–6.88
1-hexanol	–0.84	–5.38	–6.21	–6.21	–5.82	–6.06	–6.20
o-cresol	–1.06	–6.09	–7.15	–7.15	–7.11	–7.10	–7.45
1-heptanol	–0.84	–6.05	–6.88	–6.88	–6.43	–6.70	–7.10
ethanoic acid	–2.56	–2.21	–4.76	–4.76	–4.75	–4.78	–4.54
p-bromophenol	–1.24	–7.32	–8.56	–8.49	–8.42	–8.37	–8.49
Solvent: bromoethane							
n-octane	0.00	–5.03	–5.03	–5.03	–4.99	–4.95	–5.54
toluene	–0.62	–4.83	–5.46	–5.46	–6.31	–5.96	–5.55
1,4-dioxane	–2.24	–3.17	–5.40	–5.40	–5.60	–5.39	–5.39
butanone	–1.88	–2.90	–4.79	–4.79	–5.26	–5.17	–5.13
propanoic acid	–2.73	–2.91	–5.64	–5.64	–5.97	–5.88	–5.52
Solvent: dibromoethane							
methanol	–0.99	–1.51	–2.50	–2.50	–2.46	–2.47	–2.38
ethanol	–0.87	–2.47	–3.34	–3.34	–3.42	–3.38	–2.69
1-propanol	–0.84	–3.12	–3.96	–3.96	–3.92	–3.94	–3.82
1-butanol	–0.84	–3.77	–4.61	–4.61	–4.43	–4.52	–4.65
1-pentanol	–0.83	–4.39	–5.23	–5.23	–4.99	–5.10	–5.44
phenol	–1.09	–5.46	–6.56	–6.56	–6.67	–6.56	–7.22
1-hexanol	–0.88	–4.97	–5.85	–5.85	–5.57	–5.75	–6.08
p-cresol	–1.09	–5.79	–6.88	–6.88	–6.99	–6.93	–7.52
1-heptanol	–0.88	–5.59	–6.47	–6.47	–6.14	–6.34	–6.64
p-bromophenol	–1.30	–6.92	–8.23	–8.16	–8.29	–8.14	–9.01

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
Solvent: bromooctane							
methyl ethanoate	–2.58	–1.34	–3.91	–3.91	–4.15	–3.99	–3.35
ethyl ethanoate	–2.51	–2.20	–4.71	–4.71	–4.88	–4.76	–3.97
propyl ethanoate	–2.46	–2.83	–5.30	–5.30	–5.39	–5.34	–4.48
butyl ethanoate	–2.43	–3.45	–5.88	–5.88	–5.95	–5.92	–5.11
pentyl ethanoate	–2.42	–4.07	–6.49	–6.49	–6.53	–6.52	–5.81
Solvent: hexadecyliodide							
n-pentane	0.00	–2.65	–2.66	–2.66	–2.61	–2.59	–2.59
n-hexane	0.00	–3.26	–3.26	–3.26	–3.19	–3.17	–3.26
n-heptane	0.00	–3.87	–3.87	–3.87	–3.77	–3.76	–3.90
cyclohexane	0.00	–3.76	–3.76	–3.76	–3.95	–3.77	–3.66
methylcyclohexane	0.00	–3.96	–3.96	–3.96	–4.06	–3.93	–4.07
benzene	–0.45	–4.24	–4.69	–4.69	–4.82	–4.78	–3.71
toluene	–0.48	–4.56	–5.04	–5.04	–5.20	–5.16	–4.41
dichloromethane	–1.08	–1.87	–2.95	–3.26	–3.18	–2.27	–2.76
trichloromethane	–0.55	–2.91	–3.47	–3.55	–3.80	–3.22	–3.36
Solvent: fluorobenzene							
n-octane	0.00	–5.23	–5.23	–5.23	–5.37	–5.25	–4.99
toluene	–0.56	–5.00	–5.56	–5.56	–6.27	–5.98	–5.27
ethanol	–0.90	–2.44	–3.33	–3.33	–3.61	–3.46	–3.45
1,4-dioxane	–2.03	–3.29	–5.32	–5.32	–5.50	–5.38	–5.18
butanone	–1.67	–3.01	–4.68	–4.68	–5.12	–5.02	–4.60
Solvent: chlorobenzene							
n-octane	0.00	–5.00	–5.01	–5.01	–5.11	–5.00	–5.16
toluene	–0.57	–4.89	–5.46	–5.46	–6.14	–5.87	–5.18
methanol	–1.03	–1.26	–2.29	–2.29	–2.38	–2.32	–2.44
ethanol	–0.91	–2.26	–3.17	–3.17	–3.42	–3.29	–3.30
1-propanol	–0.88	–2.96	–3.83	–3.83	–4.01	–3.92	–3.82
1-butanol	–0.87	–3.66	–4.53	–4.53	–4.60	–4.56	–4.31
1-pentanol	–0.87	–4.33	–5.19	–5.19	–5.25	–5.22	–5.25

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
phenol	–1.14	–5.39	–6.53	–6.53	–7.02	–6.73	–6.96
1-hexanol	–0.91	–4.97	–5.88	–5.88	–5.93	–5.95	–5.98
o-cresol	–1.15	–5.75	–6.91	–6.91	–7.50	–7.19	–7.33
p-cresol	–1.14	–5.77	–6.91	–6.91	–7.44	–7.18	–7.23
1-heptanol	–0.91	–5.64	–6.55	–6.55	–6.59	–6.61	–6.78
1,4-dioxane	–2.05	–3.18	–5.24	–5.24	–5.37	–5.28	–5.08
propanone	–1.90	–2.20	–4.10	–4.10	–4.38	–4.37	–3.86
butanone	–1.69	–2.87	–4.56	–4.56	–4.98	–4.90	–4.47
2-pentanone	–1.68	–3.50	–5.18	–5.18	–5.49	–5.45	–5.29
2-hexanone	–1.55	–4.18	–5.74	–5.74	–6.10	–6.02	–5.84
3,3-dimethylbutanone	–1.58	–3.28	–4.86	–4.86	–5.25	–5.14	–5.25
2-heptanone	–1.66	–4.83	–6.49	–6.49	–6.82	–6.77	–6.46
propanoic acid	–2.48	–2.74	–5.22	–5.22	–5.53	–5.43	–4.38
methyl ethanoate	–2.67	–1.47	–4.14	–4.14	–4.48	–4.28	–4.00
methyl propanoate	–2.40	–2.15	–4.56	–4.56	–4.90	–4.71	–4.55
ethyl ethanoate	–2.60	–2.40	–5.00	–5.00	–5.28	–5.12	–4.63
propyl ethanoate	–2.55	–3.08	–5.63	–5.63	–5.86	–5.76	–5.15
methyl pentanoate	–2.31	–3.46	–5.78	–5.78	–6.03	–5.89	–5.83
butyl ethanoate	–2.52	–3.75	–6.27	–6.27	–6.48	–6.40	–5.74
pentyl ethanoate	–2.51	–4.42	–6.92	–6.92	–7.13	–7.06	–6.49
methylamine	–0.20	–1.86	–2.06	–2.06	–2.07	–1.96	–2.16
ethylamine	–0.18	–2.65	–2.83	–2.83	–2.81	–2.78	–2.73
dimethylamine	–0.27	–2.24	–2.51	–2.51	–2.48	–2.45	–2.75
propylamine	–0.16	–3.35	–3.51	–3.51	–3.52	–3.49	–3.59
trimethylamine	–0.39	–2.47	–2.86	–2.86	–2.99	–2.84	–2.82
butylamine	–0.16	–4.02	–4.17	–4.17	–4.19	–4.16	–4.22
aniline	–0.76	–5.55	–6.31	–6.31	–6.98	–6.78	–6.72
ammonia	–0.15	–1.47	–1.62	–1.62	–1.82	–1.47	–1.22
p-bromophenol	–1.36	–6.87	–8.23	–8.16	–8.69	–8.34	–8.54

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
Solvent: bromobenzene							
n-octane	0.00	−5.02	−5.03	−5.03	−5.08	−5.00	−5.02
toluene	−0.56	−4.95	−5.51	−5.51	−6.08	−5.86	−5.13
methanol	−1.02	−1.31	−2.33	−2.33	−2.38	−2.35	−2.31
ethanol	−0.89	−2.33	−3.22	−3.22	−3.44	−3.33	−3.26
1-propanol	−0.86	−3.03	−3.90	−3.90	−4.03	−3.96	−3.74
1-butanol	−0.86	−3.73	−4.59	−4.59	−4.62	−4.61	−4.08
1-pentanol	−0.85	−4.41	−5.26	−5.26	−5.26	−5.26	−5.06
phenol	−1.12	−5.53	−6.64	−6.64	−7.02	−6.78	−6.87
1-hexanol	−0.90	−5.05	−5.95	−5.95	−5.95	−6.00	−5.92
o-cresol	−1.14	−5.88	−7.02	−7.02	−7.49	−7.23	−7.26
p-cresol	−1.12	−5.90	−7.03	−7.03	−7.42	−7.23	−7.12
1-heptanol	−0.90	−5.73	−6.63	−6.63	−6.61	−6.66	−6.68
1,4-dioxane	−2.03	−3.20	−5.22	−5.22	−5.30	−5.26	−5.02
butanone	−1.67	−2.89	−4.55	−4.55	−4.91	−4.84	−4.37
methyl ethanoate	−2.63	−1.46	−4.09	−4.09	−4.37	−4.20	−3.87
ethyl ethanoate	−2.57	−2.40	−4.97	−4.97	−5.18	−5.05	−4.57
propyl ethanoate	−2.51	−3.09	−5.60	−5.60	−5.76	−5.69	−4.93
butyl ethanoate	−2.48	−3.76	−6.24	−6.24	−6.38	−6.33	−5.58
pentyl ethanoate	−2.47	−4.43	−6.91	−6.91	−7.04	−7.00	−6.35
ethylamine	−0.18	−2.69	−2.87	−2.87	−2.83	−2.82	−2.73
propylamine	−0.16	−3.40	−3.56	−3.56	−3.53	−3.53	−3.57
butylamine	−0.15	−4.07	−4.23	−4.23	−4.20	−4.20	−4.19
aniline	−0.75	−5.66	−6.41	−6.41	−6.96	−6.82	−6.66
p-bromophenol	−1.34	−7.02	−8.36	−8.29	−8.70	−8.41	−8.49
Solvent: iodobenzene							
n-octane	0.00	−5.03	−5.04	−5.04	−5.03	−4.98	−4.72
toluene	−0.53	−5.04	−5.58	−5.58	−5.91	−5.80	−4.99
methanol	−0.97	−1.38	−2.35	−2.35	−2.34	−2.35	−2.18

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
ethanol	–0.85	–2.42	–3.27	–3.27	–3.41	–3.35	–3.18
1-propanol	–0.82	–3.13	–3.95	–3.95	–4.01	–3.99	–3.52
1-butanol	–0.82	–3.84	–4.66	–4.66	–4.61	–4.64	–4.05
1-pentanol	–0.81	–4.52	–5.33	–5.33	–5.26	–5.30	–5.02
phenol	–1.06	–5.72	–6.79	–6.79	–6.91	–6.80	–6.76
1-hexanol	–0.86	–5.17	–6.02	–6.02	–5.94	–6.03	–5.71
o-cresol	–1.08	–6.07	–7.16	–7.16	–7.37	–7.23	–7.14
m-cresol	–1.09	–6.08	–7.18	–7.18	–7.36	–7.25	–6.04
p-cresol	–1.07	–6.09	–7.16	–7.16	–7.31	–7.23	–7.01
1-heptanol	–0.85	–5.84	–6.70	–6.70	–6.61	–6.70	–6.53
1,4-dioxane	–1.93	–3.21	–5.14	–5.14	–5.11	–5.18	–4.94
butanone	–1.57	–2.90	–4.47	–4.47	–4.71	–4.67	–4.22
ethylamine	–0.17	–2.75	–2.92	–2.92	–2.84	–2.86	–2.73
propylamine	–0.15	–3.47	–3.62	–3.62	–3.55	–3.58	–3.54
butylamine	–0.15	–4.15	–4.29	–4.29	–4.22	–4.26	–4.13
p-bromophenol	–1.27	–7.25	–8.52	–8.45	–8.64	–8.46	–8.45
Solvent: odichlorobenzene							
methanol	–1.14	–1.11	–2.25	–2.25	–2.37	–2.29	–1.73
ethanol	–1.00	–2.11	–3.11	–3.11	–3.41	–3.25	–2.34
1-propanol	–0.97	–2.79	–3.75	–3.75	–3.95	–3.85	–3.47
1-butanol	–0.96	–3.47	–4.43	–4.43	–4.50	–4.46	–3.90
1-pentanol	–0.95	–4.12	–5.08	–5.08	–5.12	–5.09	–4.93
1-hexanol	–1.00	–4.76	–5.76	–5.76	–5.79	–5.82	–5.70
1-heptanol	–1.00	–5.41	–6.42	–6.42	–6.42	–6.46	–6.50
ethylamine	–0.20	–2.54	–2.74	–2.74	–2.71	–2.67	–2.59
propylamine	–0.18	–3.22	–3.40	–3.40	–3.38	–3.36	–3.44
butylamine	–0.17	–3.88	–4.05	–4.05	–4.03	–4.01	–4.13
Solvent: perfluorobenzene							
propanone	–1.03	–2.30	–3.33	–3.33	–3.33	–3.35	–3.82

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
2-pentanone	–0.91	–3.63	–4.54	–4.54	–4.61	–4.59	–5.10
2-hexanone	–0.84	–4.32	–5.16	–5.16	–5.29	–5.22	–5.55
3,3-dimethylbutanone	–0.86	–3.49	–4.35	–4.35	–4.52	–4.43	–5.26
2-heptanone	–0.90	–4.99	–5.89	–5.89	–6.02	–5.96	–6.15
methyl ethanoate	–1.52	–1.68	–3.20	–3.20	–3.21	–3.20	–4.23
ethyl ethanoate	–1.48	–2.60	–4.07	–4.07	–4.08	–4.08	–4.56
propyl ethanoate	–1.45	–3.29	–4.74	–4.74	–4.74	–4.75	–5.06
methyl pentanoate	–1.32	–3.71	–5.04	–5.04	–5.08	–5.06	–5.59
butyl ethanoate	–1.43	–3.97	–5.40	–5.40	–5.42	–5.43	–5.52
methyl hexanoate	–1.32	–4.40	–5.71	–5.71	–5.77	–5.74	–6.21
pentyl ethanoate	–1.43	–4.65	–6.08	–6.08	–6.12	–6.12	–6.16
Solvent: methylformamide							
n-octane	0.00	–3.06	–3.06	–3.06	–2.37	–2.65	–3.34
toluene	–0.71	–3.51	–4.22	–4.22	–4.51	–4.44	–4.34
ethanol	–1.12	–4.08	–5.20	–5.20	–5.30	–5.22	–5.12
1,4-dioxane	–2.54	–2.25	–4.79	–4.79	–4.86	–4.69	–4.86
butanone	–2.21	–2.34	–4.56	–4.56	–4.78	–4.78	–4.34
Solvent: aceticacid							
n-octane	0.00	–3.36	–3.36	–3.36	–2.80	–3.00	–3.93
toluene	–0.58	–3.38	–3.96	–3.96	–3.94	–3.98	–4.53
ethanol	–0.92	–4.52	–5.45	–5.45	–5.53	–5.47	–5.25
1,4-dioxane	–2.10	–2.56	–4.65	–4.65	–4.63	–4.61	–5.80
butanone	–1.74	–2.68	–4.42	–4.42	–4.50	–4.52	–4.80
Solvent: methoxyethanol							
n-octane	0.00	–3.12	–3.12	–3.12	–2.77	–2.90	–3.71
toluene	–0.67	–3.81	–4.48	–4.48	–4.57	–4.60	–4.49
ethanol	–1.05	–4.63	–5.68	–5.68	–5.80	–5.72	–4.71
1,4-dioxane	–2.39	–2.17	–4.56	–4.56	–4.79	–4.61	–4.91
butanone	–2.04	–2.40	–4.44	–4.44	–4.69	–4.56	–4.28

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
Solvent: tributylphosphate							
methanol	–1.11	–3.91	–5.02	–5.02	–5.08	–5.03	–4.16
ethanol	–0.97	–4.66	–5.63	–5.63	–5.91	–5.77	–4.57
1-propanol	–0.94	–5.10	–6.04	–6.04	–6.29	–6.17	–5.42
1-butanol	–0.93	–5.52	–6.45	–6.45	–6.64	–6.57	–6.28
1-pentanol	–0.93	–5.93	–6.86	–6.86	–7.09	–7.00	–6.69
1-hexanol	–0.98	–6.08	–7.06	–7.06	–7.37	–7.29	–7.68
1-heptanol	–0.97	–6.49	–7.47	–7.47	–7.83	–7.73	–7.98
ethanoic acid	–3.03	–4.77	–7.79	–7.79	–7.89	–7.79	–7.11
propanoic acid	–2.69	–5.19	–7.88	–7.88	–8.06	–7.93	–7.73
butanoic acid	–2.62	–5.58	–8.20	–8.20	–8.29	–8.22	–8.29
pentanoic acid	–2.58	–5.99	–8.57	–8.57	–8.78	–8.67	–8.82
2-methoxyethanol	–1.69	–4.91	–6.59	–6.59	–6.77	–6.72	–6.14
water	–1.29	–6.43	–7.73	–7.73	–7.65	–7.68	–4.69
ethylamine	–0.20	–3.25	–3.44	–3.44	–3.66	–3.53	–3.29
propylamine	–0.17	–3.69	–3.87	–3.87	–4.16	–4.02	–3.98
butylamine	–0.17	–4.11	–4.27	–4.27	–4.63	–4.47	–4.25
aniline	–0.81	–6.46	–7.27	–7.27	–7.30	–7.43	–7.60
Solvent: tetrahydrothiophenedioxide							
n-octane	0.00	–2.24	–2.24	–2.24	–1.69	–1.95	–2.44
toluene	–0.70	–3.63	–4.33	–4.33	–4.35	–4.44	–4.23
ethanol	–1.10	–3.48	–4.58	–4.58	–4.57	–4.56	–4.30
1,4-dioxane	–2.49	–1.49	–3.98	–3.98	–4.08	–3.97	–4.90
butanone	–2.16	–1.62	–3.77	–3.77	–3.91	–3.83	–4.09
Solvent: dimethylsulfoxide							
n-octane	0.00	–2.72	–2.72	–2.72	–2.33	–2.50	–2.84
toluene	–0.70	–3.87	–4.57	–4.57	–4.76	–4.76	–4.42
ethanol	–1.10	–3.67	–4.77	–4.77	–4.84	–4.78	–5.25
1,4-dioxane	–2.50	–1.75	–4.24	–4.24	–4.47	–4.26	–4.90

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
butanone	–2.16	–1.89	–4.05	–4.05	–4.31	–4.17	–4.23
Solvent: carbon disulfide							
n-octane	0.00	–5.13	–5.14	–5.14	–5.22	–5.11	–5.68
toluene	–0.41	–5.09	–5.49	–5.49	–5.43	–5.48	–5.39
ethanol	–0.66	–2.32	–2.97	–2.97	–3.02	–3.01	–2.95
phenol	–0.82	–5.62	–6.44	–6.44	–6.17	–6.24	–6.27
1,4-dioxane	–1.49	–3.28	–4.77	–4.77	–4.57	–4.85	–4.67
propanone	–1.31	–2.25	–3.56	–3.56	–3.50	–3.55	–3.14
butanone	–1.16	–2.94	–4.10	–4.10	–4.16	–4.15	–3.85
ethanoic acid	–1.98	–2.09	–4.07	–4.07	–4.07	–4.05	–2.98
methyl ethanoate	–1.89	–1.46	–3.35	–3.35	–3.30	–3.32	–3.67
ethyl ethanoate	–1.84	–2.43	–4.27	–4.27	–4.19	–4.22	–4.08
propyl ethanoate	–1.81	–3.13	–4.94	–4.94	–4.84	–4.90	–4.63
1-nitropropane	–3.47	–1.27	–4.74	–4.74	–5.15	–4.93	–4.50
Solvent: water							
methane	–0.01	1.44	1.43	1.43	1.50	1.48	2.00
ethane	0.00	1.22	1.22	1.22	1.19	1.26	1.83
propane	0.00	1.34	1.33	1.33	1.27	1.36	1.96
n-butane	0.00	1.49	1.49	1.49	1.46	1.53	2.08
n-pentane	0.00	1.64	1.64	1.64	1.66	1.71	2.33
n-hexane	0.00	1.80	1.79	1.79	1.87	1.89	2.49
n-heptane	0.00	1.95	1.95	1.95	2.07	2.07	2.62
n-octane	0.00	2.10	2.10	2.10	2.28	2.25	2.89
2-methylpropane	–0.01	1.68	1.67	1.67	1.57	1.67	2.32
2,2-dimethylpropane	–0.02	2.12	2.10	2.10	1.90	2.05	2.50
2-methylpentane	–0.01	1.99	1.98	1.98	2.06	2.06	2.52
2,4-dimethylpentane	–0.01	2.37	2.36	2.36	2.47	2.46	2.88
2,2,4-trimethylpentane	–0.02	2.75	2.73	2.73	2.82	2.81	2.85
cyclopropane	–0.08	0.22	0.14	0.14	0.31	0.27	0.75

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
cyclopentane	–0.01	0.71	0.70	0.70	0.58	0.74	1.20
cyclohexane	0.00	0.89	0.89	0.89	0.70	0.89	1.23
methylcyclohexane	–0.01	1.30	1.30	1.30	1.20	1.34	1.71
cis-1,2-dimethylcyclohexane	–0.01	1.70	1.68	1.68	1.69	1.76	1.58
ethene	–0.10	1.11	1.01	1.01	1.33	1.20	1.27
propene	–0.14	1.09	0.95	0.95	1.12	1.06	1.27
s-trans-1,3-butadiene	–0.30	0.95	0.65	0.65	1.20	0.97	0.61
2-methylpropene	–0.21	1.37	1.16	1.16	1.16	1.18	1.16
1-butene	–0.14	1.24	1.11	1.11	1.42	1.29	1.38
cyclopentene	–0.22	0.30	0.08	0.08	–0.05	0.06	0.56
1-pentene	–0.12	1.40	1.27	1.27	1.65	1.50	1.66
E-2-pentene	–0.16	1.25	1.09	1.09	1.29	1.21	1.34
1-hexene	–0.12	1.55	1.43	1.43	1.86	1.69	1.68
ethyne	–1.47	1.68	0.21	0.21	0.30	0.29	–0.01
propyne	–1.65	1.39	–0.26	–0.26	–0.66	–0.54	–0.31
1-butyne	–1.56	1.54	–0.02	–0.02	–0.19	–0.13	–0.16
1-pentyne	–1.51	1.69	0.18	0.18	0.22	0.18	0.01
1-hexyne	–1.49	1.85	0.36	0.36	0.42	0.37	0.29
benzene	–0.66	–0.52	–1.18	–1.18	–1.39	–1.37	–0.87
toluene	–0.71	–0.18	–0.89	–0.89	–1.17	–1.13	–0.89
ethylbenzene	–0.67	0.01	–0.66	–0.66	–0.68	–0.76	–0.80
o-xylene	–0.77	0.10	–0.67	–0.67	–1.11	–1.02	–0.90
m-xylene	–0.75	0.17	–0.58	–0.58	–0.95	–0.90	–0.84
p-xylene	–0.74	0.17	–0.57	–0.57	–0.91	–0.88	–0.81
naphthalene	–1.21	–1.34	–2.55	–2.55	–2.99	–2.92	–2.39
anthracene	–1.67	–2.14	–3.81	–3.81	–4.23	–4.25	–4.23
methanol	–1.26	–4.01	–5.28	–5.28	–5.45	–5.32	–5.11
ethanol	–1.11	–3.98	–5.10	–5.10	–5.40	–5.22	–5.01
1,2-ethanediol	–1.91	–6.99	–8.89	–8.89	–9.22	–9.29	–9.30

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
1-propanol	–1.08	–3.85	–4.93	–4.93	–5.08	–4.98	–4.83
2-propanol	–1.05	–3.72	–4.77	–4.77	–4.72	–4.72	–4.76
1-butanol	–1.07	–3.75	–4.82	–4.82	–4.79	–4.79	–4.72
2-methyl-2-propanol	–0.95	–3.16	–4.11	–4.11	–4.34	–4.20	–4.51
cyclopentanol	–0.94	–4.34	–5.29	–5.29	–5.12	–5.15	–5.49
1-pentanol	–1.06	–3.60	–4.66	–4.66	–4.58	–4.60	–4.47
phenol	–1.40	–5.06	–6.46	–6.46	–6.57	–6.43	–6.62
1-hexanol	–1.11	–3.36	–4.47	–4.47	–4.34	–4.45	–4.36
o-cresol	–1.43	–4.63	–6.06	–6.06	–6.28	–6.12	–5.87
m-cresol	–1.44	–4.69	–6.13	–6.13	–6.32	–6.19	–5.49
p-cresol	–1.40	–4.72	–6.12	–6.12	–6.25	–6.17	–6.14
1-heptanol	–1.11	–3.21	–4.32	–4.32	–4.14	–4.26	–4.24
1-octanol	–1.06	–3.12	–4.18	–4.18	–3.97	–4.04	–4.09
dimethyl ether	–1.31	–0.57	–1.88	–1.88	–1.99	–1.86	–1.92
tetrahydrofuran	–1.63	–1.56	–3.19	–3.19	–3.24	–3.11	–3.47
1,4-dioxane	–2.52	–2.79	–5.31	–5.31	–5.29	–5.33	–5.05
diethyl ether	–1.09	–0.42	–1.51	–1.51	–1.68	–1.57	–1.76
methyl propyl ether	–1.15	–0.36	–1.51	–1.51	–1.53	–1.49	–1.66
methyl isopropyl ether	–1.16	–0.22	–1.38	–1.38	–1.47	–1.38	–2.01
1,2-dimethoxyethane	–1.85	–2.19	–4.04	–4.04	–4.00	–4.08	–4.84
t-butyl methyl ether	–1.12	0.24	–0.88	–0.88	–1.01	–0.91	–2.21
anisole	–1.66	–1.68	–3.34	–3.34	–3.43	–3.24	–2.45
tetrahydropyran	–1.20	–1.36	–2.56	–2.56	–2.69	–2.57	–3.12
isopropyl ether	–1.07	0.14	–0.93	–0.93	–0.65	–0.79	–0.53
ethyl phenyl ether	–1.51	–1.58	–3.10	–3.10	–3.08	–2.98	–2.22
ethanal	–2.44	–1.37	–3.82	–3.82	–3.84	–3.88	–3.50
propanal	–2.17	–1.17	–3.34	–3.34	–3.56	–3.51	–3.44
butanal	–2.15	–1.00	–3.15	–3.15	–3.22	–3.23	–3.18
pentanal	–2.15	–0.93	–3.09	–3.09	–2.83	–3.05	–3.03

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o	ΔG_S^o
benzaldehyde	–2.57	–2.69	–5.25	–5.25	–4.99	–5.10	–4.02
octanal	–2.12	–0.37	–2.49	–2.49	–2.44	–2.50	–2.29
propanone	–2.45	–1.30	–3.75	–3.75	–3.95	–3.87	–3.85
butanone	–2.19	–1.07	–3.26	–3.26	–3.59	–3.47	–3.64
cyclopentanone	–2.12	–1.92	–4.04	–4.04	–3.94	–3.95	–4.68
2-pentanone	–2.17	–0.90	–3.07	–3.07	–3.23	–3.17	–3.53
3-pentanone	–1.94	–0.84	–2.79	–2.79	–3.21	–3.06	–3.41
2-hexanone	–2.01	–0.77	–2.79	–2.79	–2.98	–2.88	–3.29
3,3-dimethylbutanone	–2.04	–0.22	–2.26	–2.26	–2.57	–2.38	–2.89
2-heptanone	–2.14	–0.59	–2.74	–2.74	–2.83	–2.80	–3.04
4-heptanone	–1.90	–0.50	–2.40	–2.40	–2.44	–2.45	–2.93
methyl phenyl ketone	–2.73	–2.58	–5.31	–5.31	–5.09	–5.12	–4.58
5-nonanone	–1.85	–0.19	–2.04	–2.04	–2.12	–2.12	–2.67
2-octanone	–2.14	–0.42	–2.56	–2.56	–2.64	–2.62	–2.88
ethanoic acid	–3.51	–3.16	–6.68	–6.68	–6.84	–6.78	–6.70
propanoic acid	–3.12	–3.01	–6.13	–6.13	–6.29	–6.24	–6.47
butanoic acid	–3.04	–2.84	–5.88	–5.88	–5.83	–5.89	–6.36
pentanoic acid	–3.00	–2.69	–5.69	–5.69	–5.67	–5.73	–6.16
hexanoic acid	–2.99	–2.54	–5.53	–5.53	–5.44	–5.53	–6.21
methyl methanoate	–3.45	0.06	–3.40	–3.40	–3.54	–3.51	–2.78
ethyl methanoate	–3.33	0.08	–3.26	–3.26	–3.30	–3.34	–2.65
methyl ethanoate	–3.34	–0.08	–3.42	–3.42	–3.65	–3.48	–3.32
methyl propanoate	–3.01	0.07	–2.94	–2.94	–3.14	–2.99	–2.93
ethyl ethanoate	–3.27	–0.06	–3.33	–3.33	–3.41	–3.31	–3.10
methyl butanoate	–2.94	0.24	–2.70	–2.70	–2.68	–2.65	–2.83
propyl ethanoate	–3.20	0.10	–3.10	–3.10	–3.08	–3.08	–2.86
methyl pentanoate	–2.90	0.39	–2.50	–2.50	–2.50	–2.47	–2.57
butyl ethanoate	–3.16	0.25	–2.90	–2.90	–2.82	–2.86	–2.55
methyl hexanoate	–2.89	0.55	–2.35	–2.35	–2.26	–2.27	–2.49

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S	ΔG^o_S
methyl octanoate	–2.88	0.86	–2.02	–2.02	–1.87	–1.91	–2.04
pentyl ethanoate	–3.15	0.41	–2.74	–2.74	–2.61	–2.68	–2.45
methyl benzoate	–3.37	–1.31	–4.68	–4.68	–4.03	–4.15	–4.28
2-propen-1-ol	–1.11	–4.12	–5.24	–5.24	–4.81	–4.97	–5.08
2-methoxyethanol	–1.92	–5.72	–7.64	–7.64	–7.56	–7.65	–6.77
butenyne	–1.74	1.26	–0.48	–0.48	–0.29	–0.29	0.04
m-hydroxybenzaldehyde	–3.10	–7.21	–10.31	–10.31	–9.81	–9.93	–9.51
p-hydroxybenzaldehyde	–3.30	–7.14	–10.44	–10.44	–10.02	–10.11	–10.48
water	–1.48	–4.83	–6.31	–6.31	–6.31	–6.31	–6.31
hydrogen	0.00	2.34	2.34	2.34	2.34	2.35	2.33
methylamine	–0.24	–4.09	–4.33	–4.33	–4.33	–4.25	–4.56
ethylamine	–0.22	–4.11	–4.33	–4.33	–4.25	–4.29	–4.50
dimethylamine	–0.33	–3.46	–3.79	–3.79	–3.70	–3.75	–4.29
azetidine	–0.47	–4.96	–5.43	–5.43	–5.18	–5.25	–5.56
propylamine	–0.20	–4.01	–4.21	–4.21	–4.12	–4.19	–4.39
trimethylamine	–0.47	–2.27	–2.74	–2.74	–2.79	–2.73	–3.23
pyrrolidine	–0.29	–4.68	–4.97	–4.97	–4.83	–5.00	–5.48
piperazine	–0.53	–8.97	–9.49	–9.49	–9.47	–9.57	–7.40
butylamine	–0.19	–3.86	–4.05	–4.05	–3.93	–4.02	–4.29
diethylamine	–0.29	–3.24	–3.54	–3.54	–3.17	–3.46	–4.07
N-methylpiperazine	–0.65	–7.66	–8.30	–8.30	–8.29	–8.38	–7.77
piperidine	–0.26	–4.21	–4.47	–4.47	–4.37	–4.53	–5.11
pentylamine	–0.19	–3.71	–3.90	–3.90	–3.71	–3.82	–4.10
N,N'-dimethylpiperazine	–0.77	–6.38	–7.15	–7.15	–7.15	–7.22	–7.58
dipropylamine	–0.23	–3.34	–3.57	–3.57	–3.08	–3.50	–3.66
pyridine	–1.36	–2.91	–4.27	–4.27	–4.35	–4.06	–4.70
2-methylpyrazine	–1.89	–5.24	–7.13	–7.13	–7.32	–6.73	–5.57
aniline	–0.94	–4.15	–5.09	–5.09	–5.37	–5.47	–5.49
2-methylpyridine	–1.46	–2.83	–4.29	–4.29	–4.59	–4.18	–4.63

	SM5.2R/MD// HF/MIDI!			SM5.2R//HF/MIDI!			
				MNDO	AM1	PM3	Expt
Solute	ΔG_{EP}	G_{CDS}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}	ΔG^{o}_{S}
3-methylpyridine	–1.33	–2.57	–3.90	–3.90	–4.07	–3.82	–4.77
4-methylpyridine	–1.37	–2.59	–3.96	–3.96	–4.16	–3.89	–4.94
2-ethylpyrazine	–1.76	–5.07	–6.82	–6.82	–6.79	–6.37	–5.51
2,4-dimethylpyridine	–1.46	–2.49	–3.95	–3.95	–4.37	–3.98	–4.86
2,5-dimethylpyridine	–1.42	–2.48	–3.90	–3.90	–4.28	–3.91	–4.72
2,6-dimethylpyridine	–1.58	–2.65	–4.22	–4.22	–4.71	–4.20	–4.60
ethanonitrile	–1.98	–1.77	–3.75	–3.75	–3.83	–4.42	–3.89
propanonitrile	–1.72	–1.67	–3.40	–3.40	–3.30	–3.87	–3.85
butanonitrile	–1.59	–1.52	–3.12	–3.12	–2.80	–3.44	–3.64
benzonitrile	–1.79	–3.22	–5.00	–5.00	–4.15	–4.70	–4.10
nitroethane	–6.55	2.85	–3.70	–3.70	–4.17	–4.26	–3.71
1-nitropropane	–6.15	2.78	–3.36	–3.36	–3.60	–4.10	–3.34
2-nitropropane	–5.93	2.95	–2.98	–2.98	–3.58	–3.37	–3.14
1-nitrobutane	–6.03	2.94	–3.08	–3.08	–3.36	–3.87	–3.08
nitrobenzene	–5.73	1.57	–4.17	–4.17	–3.18	–4.30	–4.12
2-methyl-1-nitrobenzene	–5.40	1.71	–3.70	–3.70	–2.98	–3.73	–3.59
ethanamide	–2.28	–7.01	–9.29	–9.29	–9.74	–8.56	–9.71
E-N-methylacetamide	–4.60	–4.50	–9.11	–9.11	–9.42	–9.87	–10.00
Z-N-methylacetamide	–4.04	–4.45	–8.49	–8.49	–8.83	–9.26	–10.00
1,1-dimethyl-3-phenylurea	–3.92	–5.29	–9.21	–9.21	–9.14	–9.70	–11.87
9-methyladenine	–5.68	–7.82	–13.50	–13.50	–13.62	–13.45	–13.60
1-methylthymine	–6.46	–6.97	–13.43	–13.43	–12.90	–13.00	–10.40
2-methoxyethanamine	–1.18	–5.82	–7.00	–7.00	–6.90	–7.08	–6.55
morpholine	–1.50	–6.31	–7.81	–7.81	–7.77	–7.91	–7.17
N-methylmorpholine	–1.62	–5.00	–6.62	–6.62	–6.63	–6.71	–6.34
ammonia	–0.18	–4.55	–4.73	–4.73	–5.02	–4.61	–4.29
hydrazine	–0.21	–9.09	–9.30	–9.30	–9.30	–9.30	–9.30
methanethiol	–0.13	–0.54	–0.67	–0.72	–0.74	–0.76	–1.24
ethanethiol	–0.16	–0.54	–0.69	–0.74	–0.81	–0.77	–1.30