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Supporting Information for "A Universal Quantum Mechanical Model for Solvation Free Energies Based on Gas-Phase Geometries"

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Gregory D. Hawkins, Christopher J. Cramer*, and Donald G. Truhlar*
Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455-0431

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Contents:

Table S1. Surface Tension Coefficients (cal mol^{-1} $Å^{-2}$) Optimized for SM5.2R/M.

k	$\hat{\sigma}_k^{(n)}$	$\hat{\sigma}_k^{(\alpha)}$	$\hat{\sigma}_k^{(\beta)}$	$\hat{\sigma}_k^{(\text{water})}$
H	41.39			98.86
C	47.12	29.65	–23.44	66.41
N	-19.53	–165.99	36.92	–193.07
O	–66.62	–61.40		–237.31
F	11.29			54.45
S	–77.54	–60.07	40.27	–101.80
Cl	–29.56			4.60
Br	–42.50			–13.88
I	–52.03			–35.76
H,C	–97.57			–127.61
H, N	–102.16		–158.03	–240.72
H, N (2)	–152.04			–134.82
H,O	–66.24	–330.88	–472.23	–412.19
H, O (2)	153.33			320.76
H,S	38.37			19.84
C,C	–64.18			–63.08
C, C (2)	16.89			29.16
O,C	42.50		–32.88	158.83
O,O	14.83	146.52	8.66	152.86
C, N	–60.77	218.33		122.14
N,C	–13.01	–62.52	3.61	–71.45
N, C (2)				–383.81
O,N	102.50	86.06	81.05	382.00

S,S	–0.27		35.02

$\sigma_{CS}^{(\gamma)}$	$\sigma_{CS}^{(\beta^2)}$	$\sigma_{CS}^{(\phi^2)}$	$\sigma_{CS}^{(\psi^2)}$
0.2424	10.99	–2.75	–10.07

Table S2. Surface Tension Coefficients (cal mol^{-1} $Å^{-2}$) Optimized for SM5.2R/AM1.

k	$\hat{\sigma}_k^{(n)}$	$\hat{\sigma}_k^{(\alpha)}$	$\hat{\sigma}_k^{(\beta)}$	$\hat{\sigma}_k^{(\text{water})}$
H	39.69			98.81
C	74.59	36.30	8.88	121.09
N	–31.61	–192.96	37.73	–206.82
O	–47.20	–66.98		–193.93
F	3.97			44.69
S	–73.99	–29.11	29.83	–87.33
Cl	–35.21			–4.00
Br	–47.82			–26.68
I	–54.85			–38.43
H,C	–113.40			–158.54
H, N	–95.52		–128.35	–232.98
H, N (2)	–142.74			–113.59
H,O	–89.82	–341.94	–420.35	–465.86
H, O (2)	174.52			392.05
H,S	34.13			–0.40
C,C	–68.15			–61.48
C, C (2)	3.99			16.10
O,C	20.16		–16.56	120.71
O,O	7.19	153.66	6.25	142.17
C, N	–63.46	305.33		136.46
N,C	–10.87	–72.27	–3.25	–68.86
N, C (2)				–447.64
O,N	76.85	149.02	69.91	342.64

S,S	0.01		40.62

$\sigma_{CS}^{(\gamma)}$	$\sigma_{CS}^{(\beta^2)}$	$\sigma_{CS}^{(\phi^2)}$	$\sigma_{CS}^{(\psi^2)}$
0.3024	2.47	–3.69	–8.39

Table S3. Surface Tension Coefficients (cal mol^{-1} $Å^{-2}$) Optimized for SM5.2R/PM3.

k	$\hat{\sigma}_k^{(n)}$	$\hat{\sigma}_k^{(\alpha)}$	$\hat{\sigma}_k^{(\beta)}$	$\hat{\sigma}_k^{(\text{water})}$
H	40.75			98.97
C	58.59	33.73	–6.55	90.33
N	–31.36	–179.29	30.01	–206.45
O	–72.89	–68.61		–246.03
F	1.91			39.00
S	–75.01	–41.03	34.65	–82.73
Cl	–34.69			–6.02
Br	–46.18			–21.47
I	–46.03			–10.01
H,C	–104.97			–141.97
H, N	–95.35		–134.64	–234.59
H, N (2)	–154.69			–136.37
H,O	–51.43	–329.45	–444.54	–384.85
H, O (2)	157.32			341.53
H,S	29.99			–30.98
C,C	–64.41			–59.89
C, C (2)	14.40			31.28
O,C	63.15		2.78	215.68
O,O	7.57	157.33	–9.38	129.32
C, N	–53.00	269.16		142.06
N,C	–15.18	–72.73	-1.17	–77.01
N, C (2)				–330.58
O,N	131.78	105.13	98.79	442.77

S,S	4.49		35.26

$\sigma_{CS}^{(\gamma)}$	$\sigma_{CS}^{(\beta^2)}$	$\sigma_{CS}^{(\phi^2)}$	$\sigma_{CS}^{(\psi^2)}$
0.2706	6.35	–3.27	–9.19

Table S4. Calculated and Experimental Free Energies of Solvation, ΔG_S^o (kcal/mol), for All Neutral Solutes Used in the Parameterizations of the SM5.2R Model.

	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: pentane				
methanol	–0.54	–1.09	–1.63	–1.63	–1.61	–1.65	–1.29
ethanol	–0.47	–2.04	–2.51	–2.51	–2.63	–2.59	–2.15
1-propanol	–0.46	–2.71	–3.17	–3.17	–3.30	–3.25	–2.76
1-butanol	–0.46	–3.39	–3.85	–3.85	–3.96	–3.92	–3.77
1-pentanol	–0.46	–4.04	–4.50	–4.50	–4.65	–4.58	–3.92
phenol	–0.59	–4.88	–5.47	–5.47	–5.30	–5.33	–5.67
1-hexanol	–0.48	–4.69	–5.17	–5.17	–5.35	–5.30	–4.97
1-heptanol	–0.48	–5.34	–5.82	–5.82	–6.04	–5.96	–5.62
2-pentanone	–0.80	–3.44	–4.24	–4.24	–4.37	–4.30	–4.16
2-hexanone	–0.74	–4.10	–4.84	–4.84	–5.04	–4.92	–4.79
3,3-dimethylbutanone	–0.76	–3.29	–4.05	–4.05	–4.28	–4.15	–4.43
2-heptanone	–0.79	–4.74	–5.53	–5.53	–5.75	–5.62	–5.40
methyl ethanoate	–1.35	–1.55	–2.90	–2.90	–2.93	–2.92	–3.13
methyl propanoate	–1.22	–2.21	–3.43	–3.43	–3.51	–3.48	–3.69
ethyl ethanoate	–1.31	–2.43	–3.75	–3.75	–3.79	–3.77	–3.69
propyl ethanoate	–1.29	–3.10	–4.38	–4.38	–4.45	–4.43	–4.21
methyl pentanoate	–1.18	–3.49	–4.67	–4.67	–4.79	–4.73	–4.96
butyl ethanoate	–1.27	–3.74	–5.02	–5.02	–5.12	–5.08	–4.88
methyl hexanoate	–1.17	–4.14	–5.32	–5.32	–5.47	–5.39	–5.67
pentyl ethanoate	–1.27	–4.39	–5.66	–5.66	–5.81	–5.75	–5.62
ethylamine	–0.10	–2.49	–2.58	–2.58	–2.62	–2.63	–2.18
propylamine	–0.09	–3.17	–3.26	–3.26	–3.35	–3.33	–3.13
butylamine	–0.08	–3.82	–3.90	–3.90	–4.05	–4.00	–3.62
aniline	–0.39	–5.12	–5.52	–5.52	–5.50	–5.56	–5.15
trichloromethane	–0.33	–3.17	–3.49	–3.45	–3.86	–3.48	–3.26
tribromomethane	–0.07	–5.41	–5.48	–5.40	–5.80	–5.68	–4.83

	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: hexane				
n-octane	0.00	–4.87	–4.87	–4.87	–5.20	–4.98	–5.46
benzene	–0.28	–4.22	–4.50	–4.50	–4.44	–4.47	–3.96
toluene	–0.30	–4.60	–4.90	–4.90	–4.89	–4.90	–4.84
ethylbenzene	–0.28	–5.18	–5.47	–5.47	–5.42	–5.44	–4.99
o-xylene	–0.33	–4.97	–5.30	–5.30	–5.40	–5.36	–5.22
m-xylene	–0.32	–4.97	–5.29	–5.29	–5.35	–5.34	–4.99
p-xylene	–0.31	–4.97	–5.28	–5.28	–5.34	–5.33	–5.01
methanol	–0.56	–1.06	–1.61	–1.61	–1.58	–1.63	–1.49
ethanol	–0.49	–2.00	–2.49	–2.49	–2.60	–2.56	–2.61
1-propanol	–0.47	–2.67	–3.14	–3.14	–3.25	–3.21	–2.81
1-butanol	–0.47	–3.34	–3.81	–3.81	–3.90	–3.87	–3.77
1-pentanol	–0.47	–3.98	–4.45	–4.45	–4.57	–4.52	–4.38
phenol	–0.60	–4.85	–5.46	–5.46	–5.28	–5.31	–5.49
1-hexanol	–0.49	–4.62	–5.11	–5.11	–5.26	–5.23	–5.14
o-cresol	–0.61	–5.22	–5.83	–5.83	–5.74	–5.74	–6.25
p-cresol	–0.61	–5.24	–5.85	–5.85	–5.72	–5.75	–5.86
1-heptanol	–0.49	–5.26	–5.75	–5.75	–5.94	–5.88	–5.75
1,4-dioxane	–1.11	–3.08	–4.19	–4.19	–4.09	–4.33	–4.08
benzaldehyde	–1.02	–4.95	–5.96	–5.96	–5.55	–5.73	–5.53
propanone	–0.94	–2.13	–3.07	–3.07	–3.07	–3.08	–2.60
butanone	–0.83	–2.77	–3.60	–3.60	–3.72	–3.67	–3.48
2-hexanone	–0.76	–4.03	–4.80	–4.80	–4.97	–4.87	–4.68
3,3-dimethylbutanone	–0.78	–3.21	–3.99	–3.99	–4.21	–4.09	–4.34
2-heptanone	–0.82	–4.66	–5.47	–5.47	–5.67	–5.56	–5.36
methyl phenyl ketone	–1.05	–5.63	–6.69	–6.69	–6.34	–6.46	–6.05
ethanoic acid	–1.45	–1.80	–3.25	–3.25	–3.31	–3.25	–2.83
propanoic acid	–1.29	–2.46	–3.75	–3.75	–3.86	–3.77	–2.98
methyl ethanoate	–1.39	–1.49	–2.88	–2.88	–2.90	–2.89	–3.12

	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
methyl propanoate	–1.25	–2.15	–3.40	–3.40	–3.46	–3.43	–3.65
ethyl ethanoate	–1.35	–2.37	–3.72	–3.72	–3.75	–3.73	–3.62
propyl ethanoate	–1.32	–3.02	–4.34	–4.34	–4.39	–4.38	–4.10
methyl pentanoate	–1.21	–3.41	–4.62	–4.62	–4.71	–4.67	–4.94
butyl ethanoate	–1.31	–3.66	–4.97	–4.97	–5.05	–5.02	–4.86
methyl hexanoate	–1.21	–4.05	–5.25	–5.25	–5.38	–5.31	–5.64
pentyl ethanoate	–1.30	–4.30	–5.61	–5.61	–5.72	–5.68	–5.52
p-hydroxybenzaldehyde	–1.34	–5.55	–6.89	–6.89	–6.36	–6.55	–9.18
ethylamine	–0.10	–2.45	–2.55	–2.55	–2.58	–2.59	–2.09
propylamine	–0.09	–3.13	–3.21	–3.21	–3.29	–3.28	–3.13
butylamine	–0.09	–3.77	–3.86	–3.86	–3.97	–3.94	–3.55
pyridine	–0.57	–4.06	–4.62	–4.62	–4.55	–4.51	–3.81
aniline	–0.40	–5.09	–5.50	–5.50	–5.48	–5.54	–5.43
nitroethane	–2.67	–0.88	–3.55	–3.55	–3.97	–3.65	–3.19
1-nitrobutane	–2.48	–2.18	–4.66	–4.66	–5.13	–4.89	–4.64
nitrobenzene	–2.29	–3.72	–6.01	–6.01	–5.59	–5.84	–6.09
fluorobenzene	–0.81	–3.47	–4.27	–4.30	–3.86	–4.04	–4.15
trichloromethane	–0.34	–3.13	–3.47	–3.43	–3.82	–3.44	–3.17
chlorobenzene	–0.44	–4.89	–5.33	–5.33	–5.12	–5.23	–5.14
p-dichlorobenzene	–0.43	–5.56	–5.99	–5.98	–5.66	–5.93	–5.69
tribromomethane	–0.07	–5.39	–5.47	–5.39	–5.77	–5.66	–4.38
bromobenzene	–0.40	–5.63	–6.03	–5.98	–5.93	–5.92	–5.66
p-bromophenol	–0.72	–6.24	–6.96	–6.89	–6.82	–6.80	–6.96
3,5-diBr-4-hydroxybenzonitrile	–0.75	–8.19	–8.94	–8.79	–8.32	–8.61	–9.67
Solvent: heptane							
benzene	–0.29	–4.20	–4.49	–4.49	–4.42	–4.45	–4.00
toluene	–0.31	–4.57	–4.87	–4.87	–4.86	–4.88	–4.78
o-xylene	–0.33	–4.94	–5.27	–5.27	–5.36	–5.33	–5.52
m-xylene	–0.32	–4.93	–5.25	–5.25	–5.31	–5.30	–5.67

	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
p-xylene	–0.32	–4.93	–5.25	–5.25	–5.30	–5.30	–5.52
naphthalene	–0.50	–6.73	–7.23	–7.23	–7.09	–7.15	–7.02
anthracene	–0.69	–9.24	–9.94	–9.94	–9.64	–9.79	–10.00
methanol	–0.57	–1.03	–1.60	–1.60	–1.56	–1.61	–1.29
ethanol	–0.50	–1.98	–2.47	–2.47	–2.57	–2.54	–2.15
1-propanol	–0.48	–2.64	–3.12	–3.12	–3.22	–3.19	–3.01
1-butanol	–0.48	–3.30	–3.78	–3.78	–3.86	–3.84	–3.66
1-pentanol	–0.48	–3.94	–4.42	–4.42	–4.52	–4.48	–4.09
phenol	–0.62	–4.83	–5.45	–5.45	–5.27	–5.30	–5.32
1-hexanol	–0.50	–4.57	–5.07	–5.07	–5.20	–5.18	–4.89
o-cresol	–0.62	–5.19	–5.82	–5.82	–5.72	–5.72	–6.01
m-cresol	–0.64	–5.20	–5.83	–5.83	–5.72	–5.74	–5.01
p-cresol	–0.62	–5.21	–5.83	–5.83	–5.69	–5.73	–5.77
1-heptanol	–0.50	–5.21	–5.71	–5.71	–5.87	–5.82	–5.60
anisole	–0.71	–4.43	–5.14	–5.14	–4.89	–5.00	–5.35
benzaldehyde	–1.04	–4.92	–5.96	–5.96	–5.53	–5.72	–5.50
propanone	–0.96	–2.10	–3.05	–3.05	–3.05	–3.06	–2.61
butanone	–0.85	–2.73	–3.58	–3.58	–3.69	–3.65	–3.36
2-pentanone	–0.85	–3.33	–4.18	–4.18	–4.27	–4.22	–4.07
2-hexanone	–0.78	–3.98	–4.76	–4.76	–4.92	–4.83	–4.55
3,3-dimethylbutanone	–0.80	–3.15	–3.95	–3.95	–4.15	–4.04	–4.30
2-heptanone	–0.83	–4.60	–5.43	–5.43	–5.61	–5.51	–5.22
methyl phenyl ketone	–1.08	–5.60	–6.68	–6.68	–6.32	–6.45	–6.14
2-octanone	–0.83	–5.23	–6.06	–6.06	–6.28	–6.16	–5.68
propanoic acid	–1.31	–2.42	–3.74	–3.74	–3.84	–3.76	–4.06
butanoic acid	–1.28	–3.04	–4.32	–4.32	–4.40	–4.33	–5.05
pentanoic acid	–1.27	–3.67	–4.94	–4.94	–5.08	–4.97	–5.23
hexanoic acid	–1.26	–4.31	–5.57	–5.57	–5.74	–5.62	–6.54
methyl ethanoate	–1.41	–1.45	–2.86	–2.86	–2.87	–2.87	–2.97

	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 propanoate	–1.28	–2.10	–3.37	–3.37	–3.43	–3.40	–3.63
ethyl ethanoate	–1.38	–2.32	–3.69	–3.69	–3.71	–3.71	–3.50
propyl ethanoate	–1.35	–2.97	–4.32	–4.32	–4.34	–4.35	–4.09
methyl pentanoate	–1.23	–3.35	–4.58	–4.58	–4.66	–4.62	–4.92
butyl ethanoate	–1.34	–3.60	–4.94	–4.94	–5.00	–4.98	–4.83
methyl hexanoate	–1.23	–3.98	–5.21	–5.21	–5.32	–5.26	–5.63
pentyl ethanoate	–1.33	–4.24	–5.57	–5.57	–5.66	–5.63	–5.42
ethylamine	–0.10	–2.43	–2.53	–2.53	–2.54	–2.56	–2.09
propylamine	–0.09	–3.10	–3.19	–3.19	–3.25	–3.25	–3.03
butylamine	–0.09	–3.73	–3.82	–3.82	–3.92	–3.90	–3.44
pyridine	–0.58	–4.04	–4.62	–4.62	–4.54	–4.50	–4.28
aniline	–0.41	–5.07	–5.48	–5.48	–5.46	–5.52	–5.38
ethanonitrile	–0.79	–1.46	–2.24	–2.24	–2.33	–2.58	–2.06
benzonitrile	–0.71	–5.01	–5.72	–5.72	–5.22	–5.54	–5.33
nitrobenzene	–2.33	–3.68	–6.01	–6.01	–5.58	–5.84	–6.14
thiophene	–0.97	–3.82	–4.79	–4.57	–4.54	–4.42	–4.09
fluorobenzene	–0.82	–3.44	–4.26	–4.28	–3.83	–4.02	–4.13
chlorobenzene	–0.45	–4.87	–5.31	–5.32	–5.09	–5.21	–5.15
o-dichlorobenzene	–0.58	–5.47	–6.05	–6.07	–5.82	–5.99	–6.01
p-dichlorobenzene	–0.44	–5.53	–5.98	–5.96	–5.62	–5.90	–5.81
2,2'-dichlorobiphenyl	–0.85	–9.18	–10.03	–10.02	–9.31	–9.53	–9.22
bromobenzene	–0.40	–5.62	–6.02	–5.97	–5.91	–5.90	–5.72
p-dibromobenzene	–0.37	–7.03	–7.40	–7.29	–7.26	–7.26	–7.55
iodobenzene	–0.38	–6.33	–6.71	–6.81	–6.72	–6.19	–6.27
			Solvent: octane				
toluene	–0.31	–4.54	–4.85	–4.85	–4.84	–4.85	–4.82
methanol	–0.58	–1.01	–1.59	–1.59	–1.55	–1.60	–1.29
ethanol	–0.51	–1.95	–2.46	–2.46	–2.55	–2.52	–2.15
1-propanol	–0.49	–2.61	–3.10	–3.10	–3.19	–3.16	–2.76

	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-butanol	–0.49	–3.27	–3.76	–3.76	–3.82	–3.80	–3.69
1-pentanol	–0.49	–3.90	–4.38	–4.38	–4.47	–4.44	–4.10
phenol	–0.63	–4.81	–5.44	–5.44	–5.25	–5.29	–5.47
1-hexanol	–0.51	–4.52	–5.03	–5.03	–5.14	–5.13	–4.86
o-cresol	–0.63	–5.16	–5.80	–5.80	–5.69	–5.70	–6.16
m-cresol	–0.65	–5.17	–5.82	–5.82	–5.70	–5.72	–5.19
p-cresol	–0.63	–5.18	–5.81	–5.81	–5.67	–5.71	–6.19
1-heptanol	–0.51	–5.15	–5.66	–5.66	–5.80	–5.77	–5.56
propanone	–0.98	–2.06	–3.04	–3.04	–3.03	–3.05	–2.46
butanone	–0.87	–2.69	–3.56	–3.56	–3.67	–3.62	–3.24
2-pentanone	–0.86	–3.29	–4.15	–4.15	–4.24	–4.20	–3.97
2-hexanone	–0.80	–3.93	–4.73	–4.73	–4.88	–4.79	–4.60
3,3-dimethylbutanone	–0.81	–3.10	–3.92	–3.92	–4.10	–4.00	–4.21
2-heptanone	–0.85	–4.55	–5.40	–5.40	–5.56	–5.47	–5.25
methyl ethanoate	–1.44	–1.41	–2.85	–2.85	–2.85	–2.86	–3.06
methyl propanoate	–1.30	–2.05	–3.35	–3.35	–3.40	–3.38	–3.57
ethyl ethanoate	–1.40	–2.27	–3.68	–3.68	–3.69	–3.68	–3.48
propyl ethanoate	–1.38	–2.92	–4.29	–4.29	–4.31	–4.32	–4.09
methyl pentanoate	–1.25	–3.29	–4.54	–4.54	–4.61	–4.58	–4.86
butyl ethanoate	–1.36	–3.54	–4.91	–4.91	–4.95	–4.95	–4.80
methyl hexanoate	–1.25	–3.92	–5.17	–5.17	–5.26	–5.21	–5.53
pentyl ethanoate	–1.35	–4.17	–5.53	–5.53	–5.61	–5.58	–5.36
ethylamine	–0.10	–2.40	–2.51	–2.51	–2.51	–2.53	–2.04
propylamine	–0.09	–3.07	–3.16	–3.16	–3.21	–3.21	–3.00
butylamine	–0.09	–3.70	–3.79	–3.79	–3.87	–3.85	–3.55
diethylamine	–0.13	–3.38	–3.52	–3.52	–3.42	–3.57	–3.42
2-methylpyrazine	–0.83	–4.30	–5.13	–5.13	–5.19	–5.04	–4.70
aniline	–0.42	–5.05	–5.47	–5.47	–5.44	–5.51	–4.84
2-ethylpyrazine	–0.77	–4.89	–5.66	–5.66	–5.67	–5.57	–5.51

Solute	SM5.2R/MD// HF/MIDI! ΔG_{EP}	G_{CDS}	ΔG^o_S	SM5.2R//HF/MIDI! MNDO ΔG^o_S	AM1 ΔG^o_S	PM3 ΔG^o_S	Expt ΔG^o_S
1-nitropropane	–2.63	–1.45	–4.08	–4.08	–4.46	–4.27	–3.95
Solvent: nonane							
methanol	–0.58	–0.99	–1.58	–1.58	–1.53	–1.58	–1.29
ethanol	–0.51	–1.93	–2.44	–2.44	–2.53	–2.51	–2.15
1-propanol	–0.50	–2.58	–3.08	–3.08	–3.16	–3.13	–2.76
1-butanol	–0.49	–3.24	–3.73	–3.73	–3.78	–3.77	–3.77
1-pentanol	–0.49	–3.86	–4.35	–4.35	–4.43	–4.40	–3.92
phenol	–0.64	–4.79	–5.43	–5.43	–5.24	–5.27	–5.60
1-hexanol	–0.52	–4.48	–5.00	–5.00	–5.09	–5.09	–4.97
o-cresol	–0.64	–5.14	–5.78	–5.78	–5.67	–5.68	–6.20
1-heptanol	–0.52	–5.11	–5.62	–5.62	–5.75	–5.72	–5.62
butanone	–0.88	–2.66	–3.54	–3.54	–3.64	–3.60	–3.20
2-pentanone	–0.87	–3.25	–4.13	–4.13	–4.20	–4.17	–3.97
2-hexanone	–0.81	–3.89	–4.70	–4.70	–4.83	–4.75	–4.59
3,3-dimethylbutanone	–0.82	–3.06	–3.89	–3.89	–4.06	–3.96	–4.19
2-heptanone	–0.86	–4.50	–5.36	–5.36	–5.51	–5.43	–5.24
methyl ethanoate	–1.46	–1.38	–2.83	–2.83	–2.83	–2.84	–3.02
methyl propanoate	–1.32	–2.01	–3.33	–3.33	–3.37	–3.35	–3.50
ethyl ethanoate	–1.42	–2.24	–3.66	–3.66	–3.66	–3.66	–3.45
propyl ethanoate	–1.39	–2.88	–4.27	–4.27	–4.27	–4.29	–4.07
methyl pentanoate	–1.27	–3.24	–4.51	–4.51	–4.56	–4.54	–4.85
butyl ethanoate	–1.38	–3.50	–4.88	–4.88	–4.91	–4.91	–4.69
methyl hexanoate	–1.27	–3.86	–5.13	–5.13	–5.21	–5.17	–5.51
pentyl ethanoate	–1.37	–4.12	–5.50	–5.50	–5.56	–5.54	–5.33
ethylamine	–0.10	–2.38	–2.49	–2.49	–2.48	–2.51	–1.98
propylamine	–0.09	–3.04	–3.13	–3.13	–3.17	–3.18	–2.96
butylamine	–0.09	–3.67	–3.76	–3.76	–3.83	–3.82	–3.55
Solvent: decane							
n-octane	0.00	–4.64	–4.64	–4.64	–4.89	–4.71	–5.18

	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
benzene	–0.30	–4.14	–4.44	–4.44	–4.37	–4.41	–3.80
toluene	–0.32	–4.49	–4.81	–4.81	–4.80	–4.81	–4.65
ethylbenzene	–0.30	–5.05	–5.36	–5.36	–5.28	–5.32	–5.25
methanol	–0.59	–0.98	–1.57	–1.57	–1.53	–1.58	–1.29
ethanol	–0.52	–1.91	–2.43	–2.43	–2.52	–2.49	–2.44
1-propanol	–0.50	–2.56	–3.06	–3.06	–3.14	–3.12	–2.76
1-butanol	–0.50	–3.21	–3.71	–3.71	–3.75	–3.75	–3.77
1-pentanol	–0.50	–3.83	–4.33	–4.33	–4.39	–4.37	–3.92
phenol	–0.65	–4.77	–5.42	–5.42	–5.23	–5.27	–5.50
1-hexanol	–0.53	–4.44	–4.97	–4.97	–5.05	–5.06	–4.97
p-cresol	–0.65	–5.13	–5.78	–5.78	–5.63	–5.68	–6.00
1-heptanol	–0.53	–5.07	–5.59	–5.59	–5.70	–5.68	–5.62
1,4-dioxane	–1.18	–2.96	–4.14	–4.14	–4.01	–4.26	–3.97
propanone	–1.01	–2.02	–3.02	–3.02	–3.01	–3.04	–2.47
butanone	–0.90	–2.63	–3.53	–3.53	–3.63	–3.60	–3.30
2-pentanone	–0.89	–3.22	–4.11	–4.11	–4.18	–4.15	–3.93
2-hexanone	–0.82	–3.86	–4.68	–4.68	–4.81	–4.73	–4.61
3,3-dimethylbutanone	–0.84	–3.02	–3.86	–3.86	–4.03	–3.94	–4.15
2-heptanone	–0.88	–4.46	–5.34	–5.34	–5.48	–5.40	–5.18
methyl ethanoate	–1.48	–1.35	–2.83	–2.83	–2.83	–2.83	–2.98
methyl propanoate	–1.34	–1.98	–3.32	–3.32	–3.35	–3.34	–3.49
ethyl ethanoate	–1.45	–2.21	–3.65	–3.65	–3.65	–3.65	–3.43
propyl ethanoate	–1.42	–2.84	–4.26	–4.26	–4.25	–4.27	–4.02
methyl pentanoate	–1.29	–3.20	–4.49	–4.49	–4.53	–4.51	–4.77
butyl ethanoate	–1.40	–3.46	–4.86	–4.86	–4.88	–4.89	–4.66
methyl hexanoate	–1.29	–3.82	–5.11	–5.11	–5.17	–5.14	–5.48
pentyl ethanoate	–1.40	–4.08	–5.47	–5.47	–5.53	–5.51	–5.31
ethylamine	–0.11	–2.37	–2.47	–2.47	–2.46	–2.49	–1.92
propylamine	–0.10	–3.02	–3.11	–3.11	–3.15	–3.15	–2.96

	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
butylamine	–0.09	–3.64	–3.73	–3.73	–3.80	–3.79	–3.55
ethanamide	–0.97	–2.44	–3.41	–3.41	–3.36	–3.17	–2.85
fluorobenzene	–0.86	–3.36	–4.22	–4.24	–3.77	–3.97	–3.48
trichloroethene	–0.20	–3.13	–3.33	–3.26	–3.28	–3.46	–3.84
chlorobenzene	–0.47	–4.80	–5.26	–5.27	–5.03	–5.15	–4.93
bromobenzene	–0.42	–5.55	–5.97	–5.92	–5.86	–5.85	–5.43
Solvent: undecane							
benzene	–0.30	–4.21	–4.51	–4.51	–4.42	–4.46	–4.05
toluene	–0.32	–4.56	–4.88	–4.88	–4.85	–4.88	–4.81
ethylbenzene	–0.30	–5.14	–5.44	–5.44	–5.34	–5.39	–5.44
trichloromethane	–0.36	–3.09	–3.45	–3.42	–3.77	–3.40	–3.42
1,1,1-trichloroethane	–0.53	–3.59	–4.11	–4.05	–4.47	–4.00	–3.82
E-1,2-dichloroethene	–0.27	–2.31	–2.58	–2.60	–2.42	–2.44	–3.60
trichloroethene	–0.20	–3.19	–3.38	–3.31	–3.33	–3.51	–3.87
chlorobenzene	–0.47	–4.88	–5.35	–5.35	–5.09	–5.22	–5.12
o-dichlorobenzene	–0.61	–5.49	–6.10	–6.12	–5.82	–6.01	–6.11
tribromomethane	–0.08	–5.43	–5.51	–5.43	–5.77	–5.69	–4.84
tetrachloroethene	–0.03	–4.01	–4.04	–3.68	–3.88	–4.57	–4.63
Solvent: dodecane							
ethanol	–0.53	–1.89	–2.41	–2.41	–2.50	–2.47	–2.06
1-propanol	–0.51	–2.53	–3.04	–3.04	–3.10	–3.09	–2.74
1-butanol	–0.51	–3.17	–3.68	–3.68	–3.71	–3.72	–3.47
1-pentanol	–0.51	–3.79	–4.30	–4.30	–4.34	–4.33	–4.09
1-hexanol	–0.53	–4.40	–4.93	–4.93	–5.00	–5.01	–4.28
1-heptanol	–0.53	–5.02	–5.55	–5.55	–5.63	–5.63	–5.41
methyl phenyl ketone	–1.14	–5.49	–6.63	–6.63	–6.24	–6.39	–6.11
Solvent: pentadecane							
methyl ethanoate	–1.52	–1.26	–2.78	–2.78	–2.75	–2.77	–2.82
methyl propanoate	–1.37	–1.88	–3.25	–3.25	–3.26	–3.26	–3.35

	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}
ethyl ethanoate	–1.48	–2.11	–3.59	–3.59	–3.56	–3.58	–3.37
propyl ethanoate	–1.45	–2.73	–4.18	–4.18	–4.14	–4.18	–3.91
methyl pentanoate	–1.32	–3.07	–4.39	–4.39	–4.40	–4.40	–4.59
butyl ethanoate	–1.43	–3.34	–4.77	–4.77	–4.75	–4.78	–4.49
methyl hexanoate	–1.32	–3.68	–5.00	–5.00	–5.02	–5.01	–5.35
pentyl ethanoate	–1.43	–3.94	–5.37	–5.37	–5.38	–5.39	–5.18
	Solvent: hexadecane						
methane	0.00	0.35	0.35	0.35	0.45	0.39	0.45
ethane	0.00	–0.80	–0.80	–0.80	–0.83	–0.79	–0.67
propane	0.00	–1.46	–1.46	–1.46	–1.56	–1.48	–1.43
n-butane	0.00	–2.07	–2.07	–2.07	–2.19	–2.10	–2.20
n-pentane	0.00	–2.67	–2.68	–2.68	–2.82	–2.71	–2.95
n-hexane	0.00	–3.28	–3.28	–3.28	–3.44	–3.32	–3.64
n-heptane	0.00	–3.89	–3.89	–3.89	–4.07	–3.93	–4.33
n-octane	0.00	–4.50	–4.50	–4.50	–4.69	–4.54	–5.02
n-hexadecane	0.00	–9.35	–9.35	–9.35	–9.66	–9.40	–10.52
2-methylpropane	0.00	–1.78	–1.78	–1.78	–1.93	–1.83	–1.92
2,2-dimethylpropane	–0.01	–1.93	–1.94	–1.94	–2.16	–2.02	–2.48
2-methylpentane	0.00	–2.88	–2.88	–2.88	–3.01	–2.92	–3.48
2,4-dimethylpentane	0.00	–3.14	–3.14	–3.14	–3.28	–3.18	–3.87
2,2,4-trimethylpentane	–0.01	–3.31	–3.32	–3.32	–3.49	–3.38	–4.24
cyclopropane	–0.04	–2.43	–2.47	–2.47	–2.43	–2.40	–1.78
cyclopentane	–0.01	–3.23	–3.24	–3.24	–3.48	–3.28	–3.38
cyclohexane	0.00	–3.75	–3.75	–3.75	–4.08	–3.84	–4.04
methylcyclohexane	0.00	–3.96	–3.96	–3.96	–4.27	–4.05	–4.43
ethene	–0.05	–0.41	–0.46	–0.46	–0.19	–0.32	–0.39
propene	–0.07	–1.27	–1.34	–1.34	–1.19	–1.25	–1.29
s-trans-1,3-butadiene	–0.14	–1.73	–1.87	–1.87	–1.43	–1.63	–2.10
1-butene	–0.07	–1.88	–1.94	–1.94	–1.77	–1.84	–2.03

	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-pentene	–0.06	–2.48	–2.54	–2.54	–2.38	–2.44	–2.79
1-hexene	–0.06	–3.09	–3.15	–3.15	–3.00	–3.04	–3.51
ethyne	–0.71	0.54	–0.16	–0.16	–0.08	–0.08	–0.20
propyne	–0.77	–0.65	–1.42	–1.42	–1.60	–1.52	–1.40
1-butyne	–0.73	–1.25	–1.97	–1.97	–2.08	–2.01	–2.07
1-pentyne	–0.70	–1.86	–2.56	–2.56	–2.62	–2.56	–2.74
1-hexyne	–0.69	–2.46	–3.15	–3.15	–3.25	–3.17	–3.42
benzene	–0.31	–4.09	–4.40	–4.40	–4.33	–4.36	–3.80
toluene	–0.33	–4.42	–4.75	–4.75	–4.73	–4.75	–4.54
ethylbenzene	–0.31	–4.96	–5.28	–5.28	–5.18	–5.23	–5.15
o-xylene	–0.36	–4.75	–5.11	–5.11	–5.19	–5.17	–5.37
m-xylene	–0.35	–4.74	–5.09	–5.09	–5.13	–5.14	–5.24
p-xylene	–0.35	–4.74	–5.09	–5.09	–5.12	–5.13	–5.24
naphthalene	–0.55	–6.59	–7.14	–7.14	–7.00	–7.07	–7.29
anthracene	–0.76	–9.08	–9.84	–9.84	–9.55	–9.71	–10.32
chrysene	–0.96	–11.41	–12.37	–12.37	–11.83	–12.14	–14.10
methanol	–0.62	–0.93	–1.54	–1.54	–1.49	–1.54	–1.32
ethanol	–0.54	–1.85	–2.39	–2.39	–2.46	–2.45	–2.03
1,2-ethanediol	–0.92	–2.57	–3.50	–3.50	–3.55	–3.67	–2.81
1-propanol	–0.52	–2.49	–3.01	–3.01	–3.06	–3.05	–2.77
2-propanol	–0.51	–2.36	–2.87	–2.87	–2.81	–2.87	–2.47
1-butanol	–0.52	–3.12	–3.64	–3.64	–3.65	–3.67	–3.55
2-methyl-2-propanol	–0.46	–2.55	–3.00	–3.00	–3.12	–3.08	–2.74
cyclopentanol	–0.46	–4.10	–4.56	–4.56	–4.55	–4.55	–4.42
1-pentanol	–0.52	–3.73	–4.25	–4.25	–4.27	–4.27	–4.24
phenol	–0.67	–4.72	–5.39	–5.39	–5.19	–5.23	–5.14
1-hexanol	–0.55	–4.33	–4.87	–4.87	–4.92	–4.94	–4.92
o-cresol	–0.68	–5.04	–5.72	–5.72	–5.60	–5.62	–5.78
m-cresol	–0.69	–5.04	–5.74	–5.74	–5.60	–5.63	–5.91

	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}
p-cresol	–0.67	–5.06	–5.73	–5.73	–5.57	–5.62	–5.88
1-heptanol	–0.54	–4.94	–5.48	–5.48	–5.54	–5.55	–5.62
1-octanol	–0.52	–5.54	–6.06	–6.06	–6.14	–6.09	–6.30
1-decanol	–0.51	–6.73	–7.24	–7.24	–7.43	–7.32	–7.68
dimethyl ether	–0.63	–0.55	–1.17	–1.17	–1.04	–1.18	–1.49
tetrahydrofuran	–0.76	–2.79	–3.56	–3.56	–3.52	–3.58	–3.60
1,4-dioxane	–1.23	–2.88	–4.11	–4.11	–3.95	–4.21	–3.82
diethyl ether	–0.52	–2.26	–2.77	–2.77	–2.80	–2.86	–2.81
1,2-dimethoxyethane	–0.90	–1.98	–2.89	–2.89	–2.63	–2.98	–3.63
anisole	–0.77	–4.25	–5.02	–5.02	–4.76	–4.87	–5.35
tetrahydropyran	–0.57	–3.38	–3.96	–3.96	–4.05	–4.05	–4.08
isopropyl ether	–0.50	–3.10	–3.60	–3.60	–3.47	–3.61	–4.02
ethyl phenyl ether	–0.70	–5.07	–5.77	–5.77	–5.51	–5.63	–5.64
formaldehyde	–1.13	0.04	–1.09	–1.09	–0.79	–0.95	–0.99
ethanal	–1.06	–1.22	–2.28	–2.28	–2.13	–2.25	–1.68
propanal	–0.94	–1.85	–2.79	–2.79	–2.77	–2.82	–2.48
butanal	–0.93	–2.42	–3.35	–3.35	–3.32	–3.37	–3.10
pentanal	–0.96	–3.07	–4.03	–4.03	–3.92	–4.02	–3.89
benzaldehyde	–1.14	–4.77	–5.91	–5.91	–5.46	–5.67	–5.44
octanal	–0.91	–4.84	–5.76	–5.76	–5.83	–5.80	–5.98
propanone	–1.05	–1.94	–2.99	–2.99	–2.96	–3.00	–2.31
butanone	–0.93	–2.55	–3.48	–3.48	–3.56	–3.54	–3.12
cyclopentanone	–0.93	–3.71	–4.64	–4.64	–4.62	–4.61	–4.39
2-pentanone	–0.93	–3.12	–4.05	–4.05	–4.09	–4.08	–3.76
3-pentanone	–0.82	–3.15	–3.98	–3.98	–4.14	–4.08	–3.83
2-hexanone	–0.85	–3.74	–4.60	–4.60	–4.69	–4.64	–4.45
3,3-dimethylbutanone	–0.88	–2.90	–3.77	–3.77	–3.91	–3.84	–3.94
2-heptanone	–0.91	–4.33	–5.24	–5.24	–5.34	–5.29	–5.13
4-heptanone	–0.81	–4.30	–5.11	–5.11	–5.19	–5.15	–5.20

	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	–1.18	–5.44	–6.61	–6.61	–6.22	–6.37	–6.14
5-nonanone	–0.78	–5.51	–6.29	–6.29	–6.46	–6.37	–6.46
2-octanone	–0.91	–4.93	–5.84	–5.84	–5.97	–5.90	–5.81
ethanoic acid	–1.61	–1.64	–3.25	–3.25	–3.28	–3.24	–2.39
propanoic acid	–1.43	–2.26	–3.69	–3.69	–3.76	–3.70	–3.12
butanoic acid	–1.40	–2.84	–4.24	–4.24	–4.27	–4.23	–3.86
pentanoic acid	–1.38	–3.45	–4.83	–4.83	–4.90	–4.84	–4.61
hexanoic acid	–1.38	–4.05	–5.43	–5.43	–5.52	–5.45	–5.35
methyl methanoate	–1.59	–0.23	–1.83	–1.83	–1.71	–1.82	–1.99
ethyl methanoate	–1.53	–1.09	–2.63	–2.63	–2.52	–2.63	–2.59
methyl ethanoate	–1.54	–1.25	–2.79	–2.79	–2.77	–2.79	–2.67
methyl propanoate	–1.39	–1.87	–3.26	–3.26	–3.27	–3.27	–2.68
ethyl ethanoate	–1.50	–2.10	–3.60	–3.60	–3.57	–3.59	–3.25
methyl butanoate	–1.36	–2.46	–3.82	–3.82	–3.78	–3.80	–4.01
propyl ethanoate	–1.47	–2.72	–4.19	–4.19	–4.16	–4.19	–3.93
methyl pentanoate	–1.34	–3.06	–4.40	–4.40	–4.41	–4.41	–4.69
butyl ethanoate	–1.46	–3.32	–4.78	–4.78	–4.76	–4.79	–4.61
methyl hexanoate	–1.34	–3.67	–5.00	–5.00	–5.02	–5.01	–5.43
pentyl ethanoate	–1.45	–3.93	–5.38	–5.38	–5.38	–5.40	–5.20
ethyloctadecanoate	–1.29	–11.80	–13.09	–13.09	–13.29	–13.12	–13.69
methyl benzoate	–1.52	–4.70	–6.22	–6.22	–5.60	–5.84	–6.31
2-propen-1-ol	–0.54	–2.31	–2.85	–2.85	–2.49	–2.69	–2.73
water	–0.72	0.56	–0.17	–0.17	–0.17	–0.15	–0.35
hydrogen	0.00	1.63	1.63	1.63	1.63	1.64	1.64
ethylamine	–0.11	–2.31	–2.42	–2.42	–2.38	–2.42	–2.29
dimethylamine	–0.16	–1.99	–2.15	–2.15	–2.04	–2.15	–2.18
propylamine	–0.10	–2.94	–3.04	–3.04	–3.05	–3.07	–2.92
trimethylamine	–0.23	–2.24	–2.48	–2.48	–2.49	–2.53	–2.21
butylamine	–0.10	–3.55	–3.65	–3.65	–3.68	–3.69	–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}
diethylamine	–0.14	–3.23	–3.38	–3.38	–3.22	–3.40	–3.27
pentylamine	–0.09	–4.16	–4.25	–4.25	–4.29	–4.29	–4.28
dipropylamine	–0.11	–4.51	–4.63	–4.63	–4.49	–4.70	–4.57
pyridine	–0.63	–3.93	–4.56	–4.56	–4.48	–4.43	–4.10
aniline	–0.45	–4.95	–5.40	–5.40	–5.36	–5.44	–5.44
2-methylpyridine	–0.67	–4.34	–5.01	–5.01	–5.04	–4.94	–4.68
3-methylpyridine	–0.62	–4.26	–4.88	–4.88	–4.86	–4.82	–4.91
4-methylpyridine	–0.64	–4.26	–4.90	–4.90	–4.89	–4.84	–4.89
n-methylaniline	–0.51	–5.19	–5.70	–5.70	–5.59	–5.75	–6.19
2,4-dimethylpyridine	–0.68	–4.67	–5.35	–5.35	–5.46	–5.35	–5.52
2,5-dimethylpyridine	–0.65	–4.68	–5.33	–5.33	–5.42	–5.33	–5.52
2,6-dimethylpyridine	–0.72	–4.76	–5.48	–5.48	–5.62	–5.47	–5.27
ethanonitrile	–0.86	–1.34	–2.20	–2.20	–2.27	–2.55	–2.37
propanonitrile	–0.76	–1.94	–2.70	–2.70	–2.73	–2.98	–2.84
butanonitrile	–0.71	–2.55	–3.26	–3.26	–3.25	–3.50	–3.48
benzonitrile	–0.78	–4.88	–5.66	–5.66	–5.12	–5.46	–5.51
nitroethane	–2.98	–0.62	–3.60	–3.60	–3.99	–3.68	–3.29
1-nitropropane	–2.82	–1.26	–4.08	–4.08	–4.43	–4.26	–3.95
2-nitropropane	–2.70	–1.00	–3.69	–3.69	–4.17	–3.71	–3.47
1-nitrobutane	–2.76	–1.86	–4.62	–4.62	–5.03	–4.83	–4.66
nitrobenzene	–2.55	–3.49	–6.04	–6.04	–5.55	–5.85	–6.22
2-methyl-1-nitrobenzene	–2.36	–3.88	–6.24	–6.24	–5.90	–6.04	–6.52
ethanamide	–1.01	–2.38	–3.39	–3.39	–3.32	–3.13	–3.33
ammonia	–0.09	–1.19	–1.28	–1.28	–1.42	–1.21	–0.93
ethanethiol	–0.07	–2.29	–2.35	–2.38	–2.38	–2.42	–2.96
1-propanethiol	–0.06	–2.91	–2.98	–3.00	–2.98	–3.02	–3.66
thiophenol	–0.54	–5.30	–5.83	–5.85	–5.57	–5.72	–5.61
thiophene	–1.06	–3.71	–4.78	–4.52	–4.50	–4.36	–4.01
dimethyl sulfide	–0.05	–1.82	–1.87	–2.00	–1.88	–2.02	–3.05

	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
diethyl sulfide	–0.07	–3.47	–3.54	–3.67	–3.70	–3.73	–4.23
dipropyl sulfide	–0.06	–4.74	–4.79	–4.93	–4.91	–4.93	–5.61
hydrogen sulfide	–0.05	–1.15	–1.20	–1.11	–1.06	–1.09	–0.72
dimethyl disulfide	–0.21	–4.30	–4.51	–4.48	–4.46	–4.43	–4.84
diethyl disulfide	–0.20	–5.78	–5.99	–5.94	–5.97	–5.89	–5.74
fluoroethane	–1.11	–0.20	–1.31	–1.34	–1.22	–0.99	–0.76
fluorobenzene	–0.90	–3.28	–4.18	–4.21	–3.71	–3.91	–4.03
1-fluorohexane	–1.01	–2.66	–3.67	–3.70	–3.69	–3.42	–4.03
1-fluorooctane	–1.01	–3.87	–4.88	–4.90	–4.94	–4.63	–5.25
dichloromethane	–0.72	–1.93	–2.65	–2.81	–2.87	–2.26	–2.76
trichloromethane	–0.38	–2.98	–3.35	–3.33	–3.66	–3.27	–3.38
chloroethane	–0.69	–1.74	–2.43	–2.55	–2.50	–2.09	–2.29
1,1,1-trichloroethane	–0.55	–3.45	–4.00	–3.94	–4.33	–3.85	–3.73
1,1,2-trichloroethane	–0.81	–3.55	–4.36	–4.48	–4.67	–3.97	–4.49
1-chloropropane	–0.63	–2.38	–3.01	–3.12	–3.07	–2.69	–2.86
2-chloropropane	–0.66	–2.24	–2.90	–3.00	–3.03	–2.62	–2.69
3-chloropropene	–0.63	–2.17	–2.79	–2.89	–2.52	–2.34	–2.88
Z-1,2-dichloroethene	–0.47	–2.19	–2.66	–2.82	–2.72	–2.39	–3.33
E-1,2-dichloroethene	–0.28	–2.20	–2.48	–2.52	–2.31	–2.33	–3.11
trichloroethene	–0.20	–3.06	–3.27	–3.20	–3.19	–3.38	–4.08
chlorobenzene	–0.49	–4.74	–5.22	–5.23	–4.97	–5.10	–4.99
o-dichlorobenzene	–0.63	–5.33	–5.96	–5.99	–5.68	–5.88	–6.16
p-dichlorobenzene	–0.48	–5.38	–5.87	–5.86	–5.45	–5.77	–6.02
dibromomethane	–0.30	–3.51	–3.81	–3.94	–3.85	–3.91	–3.94
tribromomethane	–0.08	–5.30	–5.38	–5.31	–5.61	–5.54	–5.16
bromoethane	–0.46	–2.52	–2.99	–3.09	–2.91	–3.09	–2.89
1-bromopropane	–0.42	–3.16	–3.58	–3.67	–3.50	–3.64	–3.57
2-bromopropane	–0.44	–3.01	–3.45	–3.54	–3.44	–3.62	–3.26
3-bromo-propene	–0.43	–2.92	–3.35	–3.42	–2.98	–3.24	–3.42

	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
1-bromobutane	–0.41	–3.76	–4.17	–4.26	–4.12	–4.23	–4.24
1-bromo-isobutane	–0.37	–3.30	–3.67	–3.74	–3.66	–3.76	–4.04
1-bromopentane	–0.40	–4.37	–4.77	–4.86	–4.74	–4.84	–4.93
bromobenzene	–0.44	–5.50	–5.94	–5.89	–5.80	–5.81	–5.51
bromotoluene	–0.72	–5.95	–6.67	–6.74	–6.50	–6.68	–6.36
p-bromo-toluene	–0.47	–5.78	–6.24	–6.17	–6.26	–6.21	–6.19
diiodomethane	–0.04	–4.97	–5.00	–5.15	–5.21	–4.77	–5.26
iodomethane	–0.24	–2.32	–2.56	–2.48	–2.44	–2.74	–2.88
iodoethane	–0.24	–3.25	–3.48	–3.41	–3.45	–3.79	–3.51
3-iodopropene	–0.22	–3.68	–3.90	–3.87	–3.62	–3.81	–4.10
1-iodopropane	–0.21	–3.89	–4.10	–4.04	–4.08	–4.28	–4.27
1-iodobutane	–0.20	–4.49	–4.69	–4.63	–4.69	–4.86	–4.95
1-iodopentane	–0.19	–5.09	–5.29	–5.24	–5.31	–5.46	–5.63
iodobenzene	–0.42	–6.22	–6.64	–6.74	–6.62	–6.08	–6.25
bromotrichloromethane	0.00	–4.54	–4.54	–4.22	–4.80	–4.99	–4.46
1-Br-1-Cl-2,2,2-triFethane	–0.70	–1.57	–2.28	–2.32	–2.68	–2.69	–2.97
1-Br-1,2,2,2-tetraFethane	–1.19	–0.10	–1.28	–1.37	–1.57	–1.57	–1.87
tetrachloroethene	–0.03	–3.87	–3.90	–3.53	–3.71	–4.43	–4.88
1,1,2-triCl-1,2,2-triFethane	–0.39	–1.70	–2.08	–1.78	–2.39	–3.22	–2.89
2,2,2-trifluoroethanol	–1.96	–0.03	–1.99	–2.06	–2.01	–1.98	–1.67
1,1-diCl-2,2-diFethyl methyl ether	–1.15	–1.78	–2.92	–2.89	–3.25	–3.12	–3.90
2,2,2-triFethyl vinyl ether	–1.51	0.08	–1.44	–1.51	–1.12	–1.34	–1.91
Solvent: *iso*-octane							
n-pentane	0.00	–3.13	–3.13	–3.13	–3.39	–3.22	–3.21
n-hexane	0.00	–3.82	–3.82	–3.82	–4.10	–3.91	–3.08
n-octane	0.00	–5.18	–5.18	–5.18	–5.54	–5.30	–5.44
propene	–0.07	–1.55	–1.61	–1.61	–1.50	–1.54	–1.61
1-butene	–0.06	–2.23	–2.29	–2.29	–2.18	–2.22	–2.26
1-pentene	–0.06	–2.91	–2.97	–2.97	–2.89	–2.90	–2.36

	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
benzene	–0.29	–4.48	–4.77	–4.77	–4.68	–4.72	–4.01
toluene	–0.31	–4.88	–5.19	–5.19	–5.17	–5.19	–4.68
m-xylene	–0.33	–5.28	–5.60	–5.60	–5.66	–5.65	–5.12
ethanol	–0.51	–2.13	–2.63	–2.63	–2.75	–2.71	–2.44
1-propanol	–0.49	–2.84	–3.33	–3.33	–3.44	–3.40	–3.00
1-butanol	–0.49	–3.55	–4.04	–4.04	–4.14	–4.11	–3.56
1-pentanol	–0.49	–4.23	–4.72	–4.72	–4.85	–4.80	–4.17
phenol	–0.63	–5.15	–5.78	–5.78	–5.58	–5.61	–5.30
1-hexanol	–0.51	–4.91	–5.42	–5.42	–5.59	–5.55	–5.10
o-cresol	–0.63	–5.54	–6.17	–6.17	–6.06	–6.07	–5.68
p-cresol	–0.63	–5.56	–6.19	–6.19	–6.04	–6.08	–5.59
1,4-dioxane	–1.15	–3.27	–4.42	–4.42	–4.32	–4.57	–4.02
butanal	–0.86	–2.82	–3.68	–3.68	–3.71	–3.71	–3.45
pentanal	–0.89	–3.54	–4.43	–4.43	–4.42	–4.46	–4.24
propanone	–0.98	–2.26	–3.24	–3.24	–3.25	–3.25	–2.44
butanone	–0.87	–2.94	–3.81	–3.81	–3.94	–3.88	–3.40
2-pentanone	–0.86	–3.59	–4.45	–4.45	–4.57	–4.51	–4.14
2-hexanone	–0.80	–4.29	–5.08	–5.08	–5.27	–5.16	–4.72
methyl benzoate	–1.42	–5.26	–6.68	–6.68	–6.09	–6.32	–6.71
aniline	–0.42	–5.40	–5.82	–5.82	–5.79	–5.86	–5.20
1-nitropropane	–2.63	–1.65	–4.29	–4.29	–4.71	–4.48	–3.94
ethanethiol	–0.06	–2.60	–2.67	–2.69	–2.75	–2.77	–3.13
1-propanethiol	–0.06	–3.31	–3.37	–3.39	–3.46	–3.45	–3.78
trichloromethane	–0.35	–3.32	–3.67	–3.63	–4.05	–3.66	–3.06
	Solvent: cyclohexane						
propane	0.00	–1.53	–1.53	–1.53	–1.64	–1.55	–2.09
n-butane	0.00	–2.15	–2.15	–2.15	–2.29	–2.19	–2.86
n-pentane	0.00	–2.77	–2.77	–2.77	–2.94	–2.81	–3.50
n-octane	0.00	–4.63	–4.63	–4.63	–4.86	–4.69	–5.63

	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
cyclohexane	0.00	–3.83	–3.83	–3.83	–4.19	–3.94	–4.43
benzene	–0.31	–4.15	–4.46	–4.46	–4.38	–4.42	–4.19
toluene	–0.33	–4.49	–4.82	–4.82	–4.80	–4.82	–4.90
ethylbenzene	–0.31	–5.06	–5.37	–5.37	–5.28	–5.32	–4.97
o-xylene	–0.35	–4.84	–5.20	–5.20	–5.28	–5.26	–5.54
m-xylene	–0.34	–4.83	–5.18	–5.18	–5.22	–5.22	–5.52
naphthalene	–0.54	–6.67	–7.21	–7.21	–7.08	–7.14	–7.17
methanol	–0.60	–0.97	–1.57	–1.57	–1.52	–1.58	–1.29
ethanol	–0.53	–1.91	–2.43	–2.43	–2.52	–2.49	–2.59
1-propanol	–0.51	–2.55	–3.06	–3.06	–3.13	–3.12	–2.73
2-propanol	–0.50	–2.43	–2.92	–2.92	–2.89	–2.93	–2.37
1-butanol	–0.51	–3.20	–3.71	–3.71	–3.75	–3.75	–3.52
2-methyl-2-propanol	–0.45	–2.63	–3.08	–3.08	–3.21	–3.16	–2.93
1-pentanol	–0.51	–3.82	–4.33	–4.33	–4.38	–4.37	–3.61
phenol	–0.66	–4.78	–5.44	–5.44	–5.25	–5.29	–5.57
1-hexanol	–0.53	–4.44	–4.97	–4.97	–5.04	–5.05	–5.31
o-cresol	–0.66	–5.12	–5.78	–5.78	–5.67	–5.69	–6.02
m-cresol	–0.68	–5.13	–5.80	–5.80	–5.67	–5.71	–5.20
p-cresol	–0.66	–5.14	–5.80	–5.80	–5.65	–5.70	–5.89
1-heptanol	–0.53	–5.06	–5.59	–5.59	–5.68	–5.68	–6.02
1,4-dioxane	–1.20	–2.95	–4.16	–4.16	–4.02	–4.26	–4.17
diethyl ether	–0.50	–2.34	–2.85	–2.85	–2.89	–2.94	–3.03
anisole	–0.75	–4.34	–5.09	–5.09	–4.83	–4.95	–5.38
tetrahydropyran	–0.56	–3.46	–4.02	–4.02	–4.13	–4.13	–4.41
ethyl phenyl ether	–0.68	–5.17	–5.85	–5.85	–5.60	–5.72	–6.00
benzaldehyde	–1.11	–4.85	–5.96	–5.96	–5.52	–5.72	–5.71
propanone	–1.03	–2.01	–3.03	–3.03	–3.01	–3.04	–2.67
butanone	–0.91	–2.62	–3.54	–3.54	–3.63	–3.60	–3.48
2-pentanone	–0.91	–3.21	–4.12	–4.12	–4.18	–4.16	–4.19

	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
3-pentanone	–0.80	–3.24	–4.05	–4.05	–4.23	–4.16	–4.30
2-hexanone	–0.84	–3.85	–4.68	–4.68	–4.80	–4.73	–4.77
3,3-dimethylbutanone	–0.85	–3.00	–3.86	–3.86	–4.02	–3.93	–4.42
2-heptanone	–0.89	–4.45	–5.34	–5.34	–5.47	–5.40	–5.47
methyl phenyl ketone	–1.15	–5.53	–6.68	–6.68	–6.29	–6.44	–6.29
ethanoic acid	–1.58	–1.69	–3.27	–3.27	–3.31	–3.27	–1.73
propanoic acid	–1.40	–2.33	–3.73	–3.73	–3.81	–3.75	–3.78
methyl ethanoate	–1.51	–1.33	–2.83	–2.83	–2.82	–2.83	–3.06
methyl propanoate	–1.36	–1.96	–3.32	–3.32	–3.35	–3.34	–3.71
ethyl ethanoate	–1.47	–2.19	–3.66	–3.66	–3.64	–3.65	–3.56
propyl ethanoate	–1.44	–2.82	–4.26	–4.26	–4.25	–4.27	–4.36
methyl pentanoate	–1.31	–3.17	–4.49	–4.49	–4.52	–4.51	–5.04
butyl ethanoate	–1.43	–3.44	–4.86	–4.86	–4.87	–4.89	–4.94
methyl hexanoate	–1.31	–3.79	–5.11	–5.11	–5.16	–5.13	–5.75
pentyl ethanoate	–1.42	–4.06	–5.48	–5.48	–5.51	–5.51	–5.71
methyl benzoate	–1.49	–4.80	–6.29	–6.29	–5.68	–5.91	–7.01
m-hydroxybenzaldehyde	–1.39	–5.48	–6.87	–6.87	–6.28	–6.52	–6.88
p-hydroxybenzaldehyde	–1.46	–5.46	–6.92	–6.92	–6.35	–6.57	–7.19
water	–0.71	0.52	–0.18	–0.18	–0.19	–0.17	–0.39
ethylamine	–0.11	–2.36	–2.47	–2.47	–2.45	–2.48	–2.04
trimethylamine	–0.23	–2.31	–2.54	–2.54	–2.57	–2.61	–2.63
butylamine	–0.09	–3.63	–3.73	–3.73	–3.78	–3.78	–3.72
diethylamine	–0.14	–3.32	–3.46	–3.46	–3.33	–3.49	–3.61
pyridine	–0.62	–3.99	–4.61	–4.61	–4.53	–4.48	–4.30
aniline	–0.44	–5.02	–5.46	–5.46	–5.43	–5.50	–5.52
2-methylpyridine	–0.65	–4.42	–5.07	–5.07	–5.11	–5.01	–5.05
3-methylpyridine	–0.61	–4.33	–4.94	–4.94	–4.92	–4.88	–5.14
4-methylpyridine	–0.63	–4.34	–4.96	–4.96	–4.96	–4.91	–5.23
2,6-dimethylpyridine	–0.70	–4.85	–5.55	–5.55	–5.70	–5.55	–5.51

	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}
ethanonitrile	–0.84	–1.39	–2.23	–2.23	–2.30	–2.58	–1.87
benzonitrile	–0.76	–4.95	–5.71	–5.71	–5.19	–5.52	–5.54
1-nitropropane	–2.76	–1.35	–4.11	–4.11	–4.47	–4.29	–4.06
nitrobenzene	–2.49	–3.57	–6.07	–6.07	–5.60	–5.89	–6.62
2-methyl-1-nitrobenzene	–2.31	–3.98	–6.29	–6.29	–5.97	–6.10	–6.71
1-propanethiol	–0.06	–2.99	–3.05	–3.07	–3.08	–3.10	–3.12
thioanisole	–0.47	–5.73	–6.20	–6.35	–6.17	–6.34	–5.66
fluorobenzene	–0.88	–3.35	–4.23	–4.26	–3.77	–3.97	–3.59
1,1,1-trichloroethane	–0.53	–3.53	–4.06	–4.00	–4.41	–3.93	–4.08
trichloroethene	–0.20	–3.13	–3.33	–3.26	–3.27	–3.46	–4.29
chlorobenzene	–0.47	–4.81	–5.29	–5.29	–5.04	–5.17	–5.10
p-dichlorobenzene	–0.47	–5.47	–5.94	–5.93	–5.54	–5.85	–5.89
bromobenzene	–0.43	–5.57	–6.00	–5.95	–5.88	–5.87	–5.29
iodobenzene	–0.41	–6.29	–6.70	–6.80	–6.70	–6.16	–6.26
difluorodichloromethane	–0.22	–1.02	–1.24	–1.09	–1.47	–1.85	–1.81
fluorotrichloromethane	–0.12	–2.52	–2.63	–2.39	–2.86	–3.16	–2.63
2,2,2-trifluoroethanol	–1.92	–0.11	–2.02	–2.09	–2.06	–2.03	–1.53
p-bromophenol	–0.78	–6.17	–6.96	–6.89	–6.79	–6.78	–7.14
3,5-diBr-4-hydroxybenzonitrile	–0.81	–8.12	–8.93	–8.78	–8.22	–8.56	–6.83
	Solvent: decalin						
toluene	–0.35	–4.42	–4.77	–4.77	–4.77	–4.79	–4.37
phenol	–0.71	–4.74	–5.46	–5.46	–5.27	–5.31	–5.38
m-cresol	–0.73	–5.06	–5.79	–5.79	–5.67	–5.70	–5.11
p-cresol	–0.72	–5.07	–5.79	–5.79	–5.64	–5.69	–5.68
anisole	–0.82	–4.24	–5.07	–5.07	–4.81	–4.92	–5.00
methyl phenyl ketone	–1.26	–5.45	–6.71	–6.71	–6.32	–6.47	–6.23
ethanoic acid	–1.72	–1.60	–3.33	–3.33	–3.35	–3.33	–4.49
propanoic acid	–1.53	–2.23	–3.75	–3.75	–3.82	–3.77	–4.42
methyl ethanoate	–1.65	–1.19	–2.83	–2.83	–2.81	–2.83	–2.90

	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}
methyl propanoate	–1.48	–1.81	–3.29	–3.29	–3.30	–3.30	–3.50
ethyl ethanoate	–1.60	–2.04	–3.65	–3.65	–3.61	–3.63	–3.47
propyl ethanoate	–1.57	–2.66	–4.23	–4.23	–4.18	–4.22	–4.05
methyl pentanoate	–1.43	–2.99	–4.42	–4.42	–4.41	–4.42	–4.83
butyl ethanoate	–1.55	–3.26	–4.81	–4.81	–4.78	–4.82	–4.71
methyl hexanoate	–1.43	–3.59	–5.02	–5.02	–5.01	–5.02	–5.51
pentyl ethanoate	–1.55	–3.86	–5.41	–5.41	–5.39	–5.42	–5.44
methyl benzoate	–1.63	–4.68	–6.31	–6.31	–5.68	–5.92	–6.76
aniline	–0.48	–4.98	–5.45	–5.45	–5.44	–5.51	–5.78
benzonitrile	–0.83	–4.90	–5.73	–5.73	–5.18	–5.53	–5.86
nitrobenzene	–2.73	–3.46	–6.19	–6.19	–5.69	–6.00	–6.36
thioanisole	–0.52	–5.66	–6.18	–6.33	–6.15	–6.33	–5.54
fluorobenzene	–0.96	–3.27	–4.23	–4.26	–3.74	–3.95	–3.44
chlorobenzene	–0.52	–4.76	–5.28	–5.29	–5.03	–5.15	–4.61
bromobenzene	–0.47	–5.54	–6.00	–5.95	–5.88	–5.87	–5.25
iodobenzene	–0.44	–6.27	–6.71	–6.82	–6.71	–6.15	–5.96
			Solvent: benzene				
n-pentane	0.00	–3.27	–3.27	–3.27	–3.41	–3.30	–2.99
n-hexane	0.00	–3.98	–3.98	–3.98	–4.13	–4.01	–3.62
n-octane	0.00	–5.40	–5.40	–5.40	–5.57	–5.43	–5.35
cyclohexane	0.00	–4.38	–4.39	–4.39	–4.72	–4.48	–4.05
benzene	–0.34	–4.75	–5.10	–5.10	–4.93	–5.02	–4.55
toluene	–0.36	–5.17	–5.53	–5.53	–5.42	–5.50	–5.32
methanol	–0.67	–1.58	–2.25	–2.25	–2.17	–2.24	–2.58
ethanol	–0.59	–2.62	–3.21	–3.21	–3.27	–3.26	–3.42
1-propanol	–0.57	–3.36	–3.93	–3.93	–3.96	–3.96	–3.87
2-propanol	–0.56	–3.21	–3.77	–3.77	–3.69	–3.75	–3.48
1-butanol	–0.57	–4.09	–4.67	–4.67	–4.65	–4.68	–4.45
2-methyl-2-propanol	–0.50	–3.48	–3.98	–3.98	–4.07	–4.04	–3.70

	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}
1-pentanol	–0.57	–4.80	–5.37	–5.37	–5.37	–5.38	–5.10
phenol	–0.73	–5.84	–6.57	–6.57	–6.26	–6.35	–7.12
1-hexanol	–0.60	–5.47	–6.07	–6.07	–6.08	–6.13	–6.13
o-cresol	–0.74	–6.24	–6.98	–6.98	–6.75	–6.81	–7.44
m-cresol	–0.76	–6.25	–7.00	–7.00	–6.75	–6.83	–6.66
p-cresol	–0.74	–6.26	–7.00	–7.00	–6.72	–6.82	–7.35
1-heptanol	–0.59	–6.18	–6.78	–6.78	–6.81	–6.84	–6.85
1-octanol	–0.56	–6.92	–7.49	–7.49	–7.54	–7.51	–8.06
1,4-dioxane	–1.34	–3.39	–4.73	–4.73	–4.60	–4.85	–5.21
propanone	–1.16	–2.42	–3.58	–3.58	–3.53	–3.55	–3.79
butanone	–1.03	–3.12	–4.15	–4.15	–4.22	–4.18	–4.46
2-pentanone	–1.02	–3.79	–4.82	–4.82	–4.84	–4.81	–5.14
2-hexanone	–0.94	–4.52	–5.46	–5.46	–5.54	–5.47	–5.76
2-heptanone	–1.01	–5.21	–6.22	–6.22	–6.29	–6.23	–6.36
ethanoic acid	–1.77	–2.44	–4.21	–4.21	–4.20	–4.17	–4.02
propanoic acid	–1.57	–3.16	–4.74	–4.74	–4.77	–4.72	–4.75
butanoic acid	–1.54	–3.85	–5.38	–5.38	–5.36	–5.34	–5.30
pentanoic acid	–1.51	–4.55	–6.07	–6.07	–6.10	–6.05	–6.01
hexanoic acid	–1.51	–5.26	–6.77	–6.77	–6.82	–6.76	–6.94
methyl ethanoate	–1.69	–1.72	–3.41	–3.41	–3.38	–3.38	–4.04
methyl propanoate	–1.53	–2.44	–3.96	–3.96	–3.97	–3.95	–4.58
ethyl ethanoate	–1.65	–2.68	–4.33	–4.33	–4.29	–4.29	–4.53
propyl ethanoate	–1.62	–3.40	–5.02	–5.02	–4.96	–5.00	–5.21
methyl pentanoate	–1.47	–3.83	–5.30	–5.30	–5.29	–5.29	–5.83
butyl ethanoate	–1.60	–4.11	–5.71	–5.71	–5.67	–5.70	–5.78
methyl hexanoate	–1.47	–4.54	–6.01	–6.01	–6.00	–5.99	–6.47
pentyl ethanoate	–1.59	–4.82	–6.41	–6.41	–6.39	–6.41	–6.53
methyl benzoate	–1.68	–5.61	–7.29	–7.29	–6.53	–6.81	–6.27
m-hydroxybenzaldehyde	–1.56	–6.68	–8.25	–8.25	–7.48	–7.76	–9.29

	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
p-hydroxybenzaldehyde	–1.65	–6.66	–8.30	–8.30	–7.57	–7.82	–9.73
water	–0.79	–0.39	–1.18	–1.18	–1.14	–1.14	–1.71
methylamine	–0.13	–2.08	–2.21	–2.21	–2.17	–2.17	–2.66
ethylamine	–0.12	–2.90	–3.02	–3.02	–2.99	–3.03	–2.73
dimethylamine	–0.18	–2.43	–2.61	–2.61	–2.54	–2.64	–3.01
propylamine	–0.11	–3.65	–3.75	–3.75	–3.75	–3.78	–3.68
trimethylamine	–0.26	–2.65	–2.90	–2.90	–2.99	–3.01	–2.80
butylamine	–0.10	–4.36	–4.46	–4.46	–4.49	–4.50	–4.33
diethylamine	–0.16	–3.89	–4.05	–4.05	–3.90	–4.09	–4.02
piperidine	–0.14	–5.10	–5.24	–5.24	–5.35	–5.40	–5.03
dipropylamine	–0.12	–5.37	–5.50	–5.50	–5.38	–5.59	–5.09
pyridine	–0.69	–4.47	–5.17	–5.17	–5.05	–5.02	–5.28
aniline	–0.49	–5.90	–6.39	–6.39	–6.26	–6.40	–6.88
2-methylpyridine	–0.73	–4.98	–5.71	–5.71	–5.72	–5.64	–5.86
4-methylpyridine	–0.70	–4.89	–5.60	–5.60	–5.56	–5.53	–6.17
2,6-dimethylpyridine	–0.79	–5.50	–6.29	–6.29	–6.40	–6.27	–6.39
nitrobenzene	–2.81	–3.88	–6.68	–6.68	–6.17	–6.47	–7.60
1,1-dimethyl-3-phenylurea	–1.89	–8.39	–10.27	–10.27	–9.73	–10.33	–12.18
ammonia	–0.10	–1.71	–1.81	–1.81	–1.93	–1.70	–1.12
hydrazine	–0.12	–6.06	–6.17	–6.17	–6.14	–6.23	–7.05
p-bromophenol	–0.88	–7.33	–8.20	–8.13	–7.94	–7.97	–8.81
Solvent: toluene							
n-octane	0.00	–5.25	–5.25	–5.25	–5.38	–5.26	–5.38
methanol	–0.70	–1.54	–2.24	–2.24	–2.16	–2.22	–2.18
ethanol	–0.61	–2.56	–3.17	–3.17	–3.23	–3.22	–3.33
1-propanol	–0.59	–3.28	–3.88	–3.88	–3.89	–3.90	–3.71
1-butanol	–0.59	–4.00	–4.60	–4.60	–4.56	–4.59	–4.31
1-pentanol	–0.59	–4.70	–5.28	–5.28	–5.25	–5.28	–5.17
phenol	–0.76	–5.75	–6.51	–6.51	–6.23	–6.30	–6.93

	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-hexanol	–0.62	–5.35	–5.97	–5.97	–5.95	–6.01	–6.12
o-cresol	–0.77	–6.13	–6.90	–6.90	–6.70	–6.75	–7.43
p-cresol	–0.77	–6.15	–6.92	–6.92	–6.67	–6.76	–7.56
1-heptanol	–0.62	–6.04	–6.66	–6.66	–6.65	–6.70	–6.75
1,4-dioxane	–1.39	–3.31	–4.70	–4.70	–4.57	–4.80	–4.91
propanone	–1.21	–2.35	–3.56	–3.56	–3.51	–3.54	–3.59
butanone	–1.08	–3.04	–4.12	–4.12	–4.18	–4.14	–4.27
2-pentanone	–1.07	–3.69	–4.76	–4.76	–4.78	–4.76	–5.02
2-hexanone	–0.99	–4.40	–5.39	–5.39	–5.45	–5.39	–5.60
3,3-dimethylbutanone	–1.01	–3.50	–4.51	–4.51	–4.62	–4.54	–5.00
2-heptanone	–1.05	–5.08	–6.13	–6.13	–6.18	–6.14	–6.30
ethanoic acid	–1.85	–2.38	–4.23	–4.23	–4.22	–4.20	–4.00
propanoic acid	–1.64	–3.09	–4.73	–4.73	–4.75	–4.71	–4.57
butanoic acid	–1.60	–3.76	–5.36	–5.36	–5.32	–5.31	–5.24
pentanoic acid	–1.58	–4.45	–6.02	–6.02	–6.04	–6.00	–5.89
hexanoic acid	–1.57	–5.14	–6.71	–6.71	–6.73	–6.69	–6.97
methyl ethanoate	–1.76	–1.65	–3.41	–3.41	–3.38	–3.38	–3.81
methyl propanoate	–1.59	–2.35	–3.94	–3.94	–3.94	–3.92	–4.62
ethyl ethanoate	–1.72	–2.59	–4.31	–4.31	–4.26	–4.27	–4.41
propyl ethanoate	–1.69	–3.30	–4.98	–4.98	–4.92	–4.95	–5.00
methyl pentanoate	–1.53	–3.71	–5.24	–5.24	–5.21	–5.21	–5.65
butyl ethanoate	–1.67	–3.99	–5.65	–5.65	–5.60	–5.63	–5.57
methyl hexanoate	–1.53	–4.40	–5.93	–5.93	–5.90	–5.90	–6.38
pentyl ethanoate	–1.66	–4.68	–6.34	–6.34	–6.30	–6.32	–6.41
methyl benzoate	–1.75	–5.49	–7.24	–7.24	–6.50	–6.76	–7.96
water	–0.82	–0.36	–1.19	–1.19	–1.16	–1.15	–1.69
methylamine	–0.14	–2.03	–2.17	–2.17	–2.12	–2.11	–2.65
ethylamine	–0.12	–2.84	–2.97	–2.97	–2.91	–2.95	–2.67
dimethylamine	–0.19	–2.37	–2.56	–2.56	–2.48	–2.57	–2.68

	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}
propylamine	–0.11	–3.57	–3.68	–3.68	–3.65	–3.69	–3.51
trimethylamine	–0.27	–2.57	–2.84	–2.84	–2.91	–2.92	–2.71
butylamine	–0.11	–4.26	–4.37	–4.37	–4.36	–4.39	–4.43
diethylamine	–0.16	–3.80	–3.96	–3.96	–3.79	–3.98	–3.75
dipropylamine	–0.13	–5.25	–5.37	–5.37	–5.21	–5.44	–5.24
pyridine	–0.72	–4.39	–5.12	–5.12	–5.02	–4.98	–5.13
aniline	–0.51	–5.81	–6.32	–6.32	–6.22	–6.34	–6.69
1-nitropropane	–3.23	–1.30	–4.54	–4.54	–5.00	–4.77	–5.25
ammonia	–0.10	–1.68	–1.78	–1.78	–1.90	–1.67	–2.38
p-bromophenol	–0.91	–7.22	–8.13	–8.05	–7.89	–7.90	–8.70
Solvent: ethylbenzene							
methanol	–0.71	–1.52	–2.23	–2.23	–2.14	–2.21	–1.43
ethanol	–0.62	–2.53	–3.15	–3.15	–3.19	–3.18	–2.49
1-propanol	–0.60	–3.23	–3.84	–3.84	–3.83	–3.85	–3.71
1-butanol	–0.60	–3.94	–4.54	–4.54	–4.47	–4.52	–3.77
1-pentanol	–0.60	–4.61	–5.21	–5.21	–5.14	–5.18	–4.72
phenol	–0.78	–5.69	–6.47	–6.47	–6.16	–6.25	–6.82
1-hexanol	–0.63	–5.25	–5.88	–5.88	–5.81	–5.89	–5.68
o-cresol	–0.79	–6.06	–6.84	–6.84	–6.61	–6.68	–7.25
1-heptanol	–0.63	–5.93	–6.55	–6.55	–6.49	–6.56	–6.70
propanone	–1.23	–2.29	–3.52	–3.52	–3.45	–3.48	–3.41
butanone	–1.10	–2.96	–4.05	–4.05	–4.09	–4.07	–4.12
2-pentanone	–1.09	–3.60	–4.69	–4.69	–4.66	–4.66	–4.85
2-hexanone	–1.00	–4.29	–5.29	–5.29	–5.31	–5.27	–5.49
3,3-dimethylbutanone	–1.03	–3.39	–4.42	–4.42	–4.49	–4.43	–4.92
2-heptanone	–1.07	–4.95	–6.02	–6.02	–6.02	–6.00	–6.10
methyl ethanoate	–1.79	–1.57	–3.37	–3.37	–3.32	–3.32	–3.74
methyl propanoate	–1.62	–2.26	–3.88	–3.88	–3.85	–3.84	–4.29
ethyl ethanoate	–1.75	–2.50	–4.25	–4.25	–4.17	–4.19	–4.31

	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
propyl ethanoate	–1.71	–3.19	–4.91	–4.91	–4.80	–4.85	–4.95
methyl pentanoate	–1.56	–3.58	–5.14	–5.14	–5.07	–5.09	–5.56
butyl ethanoate	–1.69	–3.86	–5.56	–5.56	–5.46	–5.51	–5.48
pentyl ethanoate	–1.69	–4.54	–6.23	–6.23	–6.13	–6.18	–6.20
water	–0.83	–0.40	–1.23	–1.23	–1.20	–1.20	–1.51
ethylamine	–0.13	–2.79	–2.92	–2.92	–2.84	–2.89	–2.59
propylamine	–0.11	–3.50	–3.61	–3.61	–3.56	–3.60	–3.44
trimethylamine	–0.27	–2.49	–2.76	–2.76	–2.80	–2.82	–2.64
butylamine	–0.11	–4.18	–4.29	–4.29	–4.24	–4.28	–4.06
p-bromophenol	–0.93	–7.14	–8.07	–8.00	–7.80	–7.83	–8.54
Solvent: *iso*-propylbenzene							
ethanol	–0.61	–2.56	–3.17	–3.17	–3.19	–3.19	–2.90
propanone	–1.21	–2.29	–3.50	–3.50	–3.41	–3.44	–3.32
butanone	–1.07	–2.96	–4.03	–4.03	–4.05	–4.03	–4.02
2-pentanone	–1.06	–3.60	–4.67	–4.67	–4.62	–4.62	–4.84
2-hexanone	–0.98	–4.29	–5.27	–5.27	–5.27	–5.23	–5.39
3,3-dimethylbutanone	–1.00	–3.40	–4.40	–4.40	–4.45	–4.39	–4.81
2-heptanone	–1.05	–4.95	–6.00	–6.00	–5.98	–5.96	–5.99
propanoic acid	–1.63	–3.07	–4.71	–4.71	–4.68	–4.66	–4.23
butanoic acid	–1.60	–3.72	–5.32	–5.32	–5.23	–5.24	–4.93
methyl propanoate	–1.58	–2.27	–3.85	–3.85	–3.80	–3.80	–4.19
ethyl ethanoate	–1.71	–2.51	–4.22	–4.22	–4.12	–4.15	–4.22
propyl ethanoate	–1.68	–3.20	–4.88	–4.88	–4.75	–4.81	–4.78
methyl pentanoate	–1.53	–3.59	–5.12	–5.12	–5.02	–5.05	–5.45
butyl ethanoate	–1.66	–3.87	–5.53	–5.53	–5.40	–5.46	–5.36
methyl hexanoate	–1.52	–4.26	–5.79	–5.79	–5.69	–5.71	–6.19
pentyl ethanoate	–1.65	–4.54	–6.20	–6.20	–6.08	–6.13	–6.13
water	–0.82	–0.46	–1.28	–1.28	–1.23	–1.24	–1.41

	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
Solvent: butylbenzene							
phenol	–0.76	–5.60	–6.36	–6.36	–6.00	–6.11	–6.76
2-pentanone	–1.06	–3.50	–4.56	–4.56	–4.50	–4.52	–4.74
2-hexanone	–0.98	–4.18	–5.16	–5.16	–5.14	–5.11	–5.31
3,3-dimethylbutanone	–1.00	–3.29	–4.29	–4.29	–4.32	–4.27	–4.77
2-heptanone	–1.05	–4.82	–5.87	–5.87	–5.83	–5.82	–5.93
methyl propanoate	–1.58	–2.18	–3.76	–3.76	–3.69	–3.70	–4.19
methyl pentanoate	–1.52	–3.47	–5.00	–5.00	–4.88	–4.92	–5.37
butyl ethanoate	–1.65	–3.75	–5.41	–5.41	–5.26	–5.33	–5.28
methyl hexanoate	–1.52	–4.13	–5.65	–5.65	–5.53	–5.57	–6.09
Solvent: *sec*-butylbenzene							
methyl ethanoate	–1.74	–1.54	–3.27	–3.27	–3.19	–3.21	–3.91
ethyl ethanoate	–1.69	–2.46	–4.15	–4.15	–4.03	–4.07	–4.11
propyl ethanoate	–1.66	–3.14	–4.80	–4.80	–4.65	–4.72	–4.62
butyl ethanoate	–1.64	–3.80	–5.44	–5.44	–5.29	–5.37	–5.22
pentyl ethanoate	–1.64	–4.46	–6.10	–6.10	–5.95	–6.02	–5.98
Solvent: *t*-butylbenzene							
butanone	–1.06	–2.94	–4.00	–4.00	–4.00	–3.98	–3.94
2-pentanone	–1.05	–3.57	–4.62	–4.62	–4.56	–4.57	–4.72
2-hexanone	–0.97	–4.26	–5.23	–5.23	–5.21	–5.18	–5.27
3,3-dimethylbutanone	–0.99	–3.37	–4.36	–4.36	–4.39	–4.34	–4.79
2-heptanone	–1.04	–4.91	–5.95	–5.95	–5.91	–5.90	–5.88
methyl ethanoate	–1.74	–1.55	–3.29	–3.29	–3.21	–3.23	–3.57
methyl propanoate	–1.57	–2.24	–3.81	–3.81	–3.74	–3.75	–4.17
ethyl ethanoate	–1.69	–2.48	–4.17	–4.17	–4.05	–4.09	–4.22
propyl ethanoate	–1.66	–3.17	–4.83	–4.83	–4.68	–4.75	–4.72
methyl pentanoate	–1.51	–3.55	–5.07	–5.07	–4.95	–4.99	–5.39
butyl ethanoate	–1.64	–3.83	–5.47	–5.47	–5.33	–5.40	–5.25
methyl hexanoate	–1.51	–4.22	–5.73	–5.73	–5.61	–5.65	–6.13
pentyl ethanoate	–1.64	–4.50	–6.14	–6.14	–6.00	–6.07	–5.92

	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: xylene				
n-octane	0.00	–5.12	–5.12	–5.12	–5.18	–5.09	–5.29
toluene	–0.38	–5.00	–5.38	–5.38	–5.24	–5.33	–5.06
methanol	–0.70	–1.56	–2.26	–2.26	–2.15	–2.23	–1.73
ethanol	–0.61	–2.57	–3.18	–3.18	–3.21	–3.21	–3.32
1-propanol	–0.60	–3.27	–3.87	–3.87	–3.85	–3.87	–3.57
1-butanol	–0.59	–3.98	–4.58	–4.58	–4.49	–4.55	–4.17
1-pentanol	–0.59	–4.66	–5.25	–5.25	–5.16	–5.22	–4.72
phenol	–0.77	–5.74	–6.51	–6.51	–6.17	–6.27	–6.83
1-hexanol	–0.62	–5.30	–5.92	–5.92	–5.83	–5.92	–5.85
o-cresol	–0.78	–6.11	–6.89	–6.89	–6.62	–6.70	–7.25
m-cresol	–0.79	–6.12	–6.91	–6.91	–6.62	–6.72	–6.32
p-cresol	–0.77	–6.13	–6.90	–6.90	–6.58	–6.71	–7.18
1-heptanol	–0.62	–5.97	–6.60	–6.60	–6.51	–6.60	–6.74
1,4-dioxane	–1.40	–3.23	–4.63	–4.63	–4.46	–4.71	–4.86
propanone	–1.22	–2.30	–3.52	–3.52	–3.43	–3.46	–3.26
butanone	–1.08	–2.97	–4.05	–4.05	–4.07	–4.05	–4.23
2-pentanone	–1.07	–3.62	–4.69	–4.69	–4.65	–4.65	–4.87
2-hexanone	–0.99	–4.31	–5.30	–5.30	–5.30	–5.26	–5.49
3,3-dimethylbutanone	–1.01	–3.41	–4.42	–4.42	–4.48	–4.42	–4.91
2-heptanone	–1.06	–4.97	–6.03	–6.03	–6.01	–6.00	–6.15
ethanoic acid	–1.85	–2.39	–4.24	–4.24	–4.20	–4.19	–4.08
propanoic acid	–1.65	–3.08	–4.73	–4.73	–4.71	–4.69	–4.72
butanoic acid	–1.61	–3.74	–5.35	–5.35	–5.26	–5.27	–5.30
pentanoic acid	–1.58	–4.41	–6.00	–6.00	–5.95	–5.94	–5.71
hexanoic acid	–1.58	–5.09	–6.67	–6.67	–6.62	–6.61	–6.67
methyl ethanoate	–1.77	–1.58	–3.35	–3.35	–3.29	–3.30	–3.70
methyl propanoate	–1.60	–2.27	–3.87	–3.87	–3.82	–3.83	–4.20
ethyl ethanoate	–1.72	–2.52	–4.24	–4.24	–4.14	–4.17	–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
propyl ethanoate	–1.69	–3.21	–4.90	–4.90	–4.78	–4.84	–4.87
methyl pentanoate	–1.54	–3.60	–5.14	–5.14	–5.05	–5.08	–5.61
butyl ethanoate	–1.67	–3.88	–5.56	–5.56	–5.44	–5.50	–5.40
methyl hexanoate	–1.54	–4.28	–5.82	–5.82	–5.72	–5.75	–6.26
pentyl ethanoate	–1.66	–4.56	–6.23	–6.23	–6.11	–6.17	–6.19
water	–0.82	–0.46	–1.28	–1.28	–1.24	–1.24	–1.56
methylamine	–0.14	–2.02	–2.15	–2.15	–2.08	–2.09	–3.20
ethylamine	–0.13	–2.81	–2.94	–2.94	–2.85	–2.91	–3.01
dimethylamine	–0.19	–2.32	–2.51	–2.51	–2.40	–2.51	–3.36
propylamine	–0.11	–3.53	–3.64	–3.64	–3.58	–3.63	–3.69
trimethylamine	–0.27	–2.49	–2.76	–2.76	–2.80	–2.83	–2.63
butylamine	–0.11	–4.21	–4.31	–4.31	–4.26	–4.31	–4.22
diethylamine	–0.16	–3.73	–3.89	–3.89	–3.67	–3.89	–3.93
piperidine	–0.14	–4.93	–5.08	–5.08	–5.12	–5.20	–5.15
pentylamine	–0.11	–4.88	–4.99	–4.99	–4.94	–4.98	–4.70
dipropylamine	–0.13	–5.15	–5.27	–5.27	–5.05	–5.31	–5.35
pyridine	–0.72	–4.33	–5.06	–5.06	–4.92	–4.89	–5.12
aniline	–0.51	–5.78	–6.29	–6.29	–6.13	–6.28	–6.10
p-bromophenol	–0.91	–7.20	–8.11	–8.04	–7.81	–7.85	–8.69
Solvent: *iso*-propyltoluene							
methyl ethanoate	–1.67	–1.61	–3.27	–3.27	–3.14	–3.19	–3.32
methyl propanoate	–1.50	–2.30	–3.80	–3.80	–3.69	–3.72	–4.14
methyl pentanoate	–1.45	–3.63	–5.08	–5.08	–4.92	–4.98	–5.33
methyl hexanoate	–1.45	–4.31	–5.75	–5.75	–5.59	–5.64	–6.06
pentyl ethanoate	–1.57	–4.59	–6.16	–6.16	–5.97	–6.06	–6.02
Solvent: trimethylbenzene							
butanone	–1.07	–2.95	–4.03	–4.03	–4.00	–3.99	–3.97
2-pentanone	–1.06	–3.59	–4.66	–4.66	–4.56	–4.58	–4.83
2-hexanone	–0.98	–4.28	–5.26	–5.26	–5.20	–5.18	–5.39

	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}
3,3-dimethylbutanone	–1.00	–3.38	–4.38	–4.38	–4.38	–4.33	–4.80
2-heptanone	–1.05	–4.93	–5.98	–5.98	–5.90	–5.90	–6.01
methyl ethanoate	–1.76	–1.56	–3.32	–3.32	–3.21	–3.24	–3.58
methyl propanoate	–1.58	–2.25	–3.83	–3.83	–3.73	–3.76	–4.14
methyl pentanoate	–1.53	–3.56	–5.09	–5.09	–4.94	–4.99	–5.41
methyl hexanoate	–1.52	–4.24	–5.76	–5.76	–5.60	–5.65	–6.16
pentyl ethanoate	–1.65	–4.52	–6.17	–6.17	–5.99	–6.07	–6.09
Solvent: mesitylene							
phenol	–0.73	–5.87	–6.61	–6.61	–6.14	–6.30	–6.80
butanone	–1.03	–3.01	–4.04	–4.04	–4.00	–3.99	–3.95
2-pentanone	–1.02	–3.65	–4.68	–4.68	–4.58	–4.59	–4.80
2-hexanone	–0.94	–4.35	–5.30	–5.30	–5.24	–5.21	–5.34
3,3-dimethylbutanone	–0.97	–3.45	–4.42	–4.42	–4.42	–4.37	–4.77
2-heptanone	–1.01	–5.01	–6.02	–6.02	–5.95	–5.94	–5.99
Solvent: tetralin							
ethanol	–0.68	–2.57	–3.25	–3.25	–3.25	–3.26	–1.54
propanone	–1.36	–2.21	–3.57	–3.57	–3.46	–3.52	–2.54
butanone	–1.22	–2.86	–4.07	–4.07	–4.07	–4.07	–3.12
2-pentanone	–1.21	–3.48	–4.68	–4.68	–4.59	–4.63	–3.99
2-hexanone	–1.11	–4.15	–5.27	–5.27	–5.21	–5.21	–4.64
3,3-dimethylbutanone	–1.14	–3.24	–4.37	–4.37	–4.37	–4.34	–4.19
2-heptanone	–1.19	–4.79	–5.98	–5.98	–5.88	–5.92	–5.33
water	–0.91	–0.56	–1.47	–1.47	–1.42	–1.43	0.07
Solvent: ethanol							
n-octane	0.00	–4.03	–4.03	–4.03	–3.61	–3.75	–4.23
toluene	–0.68	–4.04	–4.73	–4.73	–5.21	–5.03	–4.57
1,4-dioxane	–2.44	–2.77	–5.21	–5.21	–5.42	–5.17	–4.68
butanone	–2.10	–2.85	–4.95	–4.95	–5.30	–5.23	–4.32
chlorobenzene	–1.05	–4.36	–5.41	–5.54	–5.53	–5.40	–3.30

Solute	SM5.2R/MD// HF/MIDI! ΔG_{ENP}	G_{CDS}	ΔG^{o}_{S}	SM5.2R//HF/MIDI! MNDO ΔG^{o}_{S}	AM1 ΔG^{o}_{S}	PM3 ΔG^{o}_{S}	Expt ΔG^{o}_{S}
Solvent: propanol							
n-octane	0.00	–4.04	–4.04	–4.04	–3.62	–3.76	–4.39
toluene	–0.68	–4.08	–4.75	–4.75	–5.18	–5.03	–4.47
ethanol	–1.07	–4.18	–5.25	–5.25	–5.43	–5.31	–5.01
1,4-dioxane	–2.42	–2.79	–5.20	–5.20	–5.37	–5.16	–4.61
butanone	–2.07	–2.85	–4.93	–4.93	–5.25	–5.18	–4.15
Solvent: *iso*-propanol							
n-octane	0.00	–4.16	–4.16	–4.16	–3.79	–3.91	–4.50
toluene	–0.67	–4.24	–4.91	–4.91	–5.30	–5.17	–4.38
ethanol	–1.06	–4.33	–5.40	–5.40	–5.58	–5.46	–4.84
1,4-dioxane	–2.40	–2.81	–5.22	–5.22	–5.43	–5.21	–4.49
butanone	–2.06	–2.91	–4.98	–4.98	–5.30	–5.21	–4.07
Solvent: butanol							
n-octane	0.00	–3.99	–4.00	–4.00	–3.55	–3.70	–4.45
benzene	–0.63	–3.78	–4.41	–4.41	–4.75	–4.62	–3.39
toluene	–0.67	–4.06	–4.73	–4.73	–5.10	–4.97	–4.50
ethylbenzene	–0.63	–4.56	–5.19	–5.19	–5.28	–5.28	–4.46
methanol	–1.20	–3.31	–4.51	–4.51	–4.55	–4.49	–4.73
ethanol	–1.05	–4.16	–5.21	–5.21	–5.38	–5.27	–5.02
1,2-ethanediol	–1.80	–6.30	–8.10	–8.10	–8.32	–8.35	–8.69
formaldehyde	–2.44	–0.45	–2.90	–2.90	–2.78	–2.85	–3.49
butanone	–2.04	–2.83	–4.87	–4.87	–5.16	–5.11	–4.12
ethanoic acid	–3.31	–3.50	–6.81	–6.81	–6.94	–6.90	–6.81
propanoic acid	–2.94	–4.06	–7.00	–7.00	–7.11	–7.09	–7.17
butanoic acid	–2.86	–4.59	–7.45	–7.45	–7.34	–7.43	–7.66
pentanoic acid	–2.82	–5.14	–7.96	–7.96	–7.85	–7.95	–8.02
hexanoic acid	–2.82	–5.69	–8.50	–8.50	–8.31	–8.45	–8.75
ethylamine	–0.21	–3.93	–4.14	–4.14	–4.08	–4.08	–4.50
propylamine	–0.19	–4.52	–4.71	–4.71	–4.62	–4.66	–5.04

	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
butylamine	–0.18	–5.07	–5.26	–5.26	–5.11	–5.18	–5.52
diethylamine	–0.28	–4.41	–4.69	–4.69	–4.39	–4.65	–5.15
Solvent: *sec*-butanol							
formaldehyde	–2.43	–0.49	–2.91	–2.91	–2.78	–2.83	–2.86
ethanoic acid	–3.29	–3.75	–7.04	–7.04	–7.15	–7.11	–6.81
propanoic acid	–2.92	–4.33	–7.25	–7.25	–7.34	–7.32	–7.00
butanoic acid	–2.84	–4.87	–7.71	–7.71	–7.60	–7.68	–7.34
pentanoic acid	–2.80	–5.43	–8.23	–8.23	–8.13	–8.22	–7.61
hexanoic acid	–2.80	–5.99	–8.79	–8.79	–8.61	–8.73	–8.11
water	–1.39	–4.69	–6.08	–6.08	–6.24	–6.16	–5.71
Solvent: *iso*-butanol							
butanal	–2.00	–2.80	–4.80	–4.80	–4.87	–4.94	–4.82
ethanoic acid	–3.30	–3.56	–6.86	–6.86	–7.01	–6.96	–6.80
propanoic acid	–2.93	–4.14	–7.07	–7.07	–7.20	–7.17	–6.98
butanoic acid	–2.86	–4.68	–7.54	–7.54	–7.45	–7.53	–7.62
pentanoic acid	–2.81	–5.25	–8.06	–8.06	–7.98	–8.07	–8.06
hexanoic acid	–2.81	–5.81	–8.62	–8.62	–8.46	–8.58	–8.77
ethyl ethanoate	–3.07	–1.85	–4.92	–4.92	–5.06	–4.90	–4.27
methylamine	–0.23	–3.26	–3.48	–3.48	–3.50	–3.39	–4.56
dimethylamine	–0.31	–3.27	–3.58	–3.58	–3.57	–3.59	–4.43
trimethylamine	–0.45	–3.00	–3.44	–3.44	–3.56	–3.50	–3.90
piperazine	–0.50	–7.75	–8.25	–8.25	–8.63	–8.55	–6.58
butylamine	–0.18	–5.17	–5.35	–5.35	–5.23	–5.29	–5.55
diethylamine	–0.28	–4.51	–4.78	–4.78	–4.51	–4.76	–4.86
piperidine	–0.24	–5.70	–5.95	–5.95	–6.02	–6.10	–6.17
dipropylamine	–0.22	–5.83	–6.04	–6.04	–5.65	–6.03	–5.87
pyridine	–1.28	–4.10	–5.38	–5.38	–5.72	–5.34	–5.87
Solvent: pentanol							
benzene	–0.62	–3.81	–4.42	–4.42	–4.73	–4.61	–3.53