Small molecule hydration free energies in explicit solvent: An extensive test of atomistic simulations: Supporting Information

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Table 1 shows the full computed ($\Delta G_{hyd.}$) and experimental ($\Delta G_{expt.}$) hydration free energies for all of the compounds in the test set with the original GAFF parameters. It includes the breakdown into electrostatic components ($\Delta G_{elec.}$) and nonpolar components ($\Delta G_{vdw.}$). Computed uncertainties are provided.

TABLE 1:: Computed and experimental hydration free energies and components.

Molecule name	$\Delta G_{elec.}$	$\Delta G_{vdw.}$	$\Delta G_{hyd.}$	$\Delta G_{expt.}$
1112_tetrachloroethane	-1.43 ± 0.01	1.54 ± 0.02	0.11 ± 0.02	-1.28
111_trichloroethane	-1.13 ± 0.00	1.88 ± 0.02	0.75 ± 0.02	-0.19
111_trifluoro_222_trimethoxyethane	-4.57 ± 0.01	2.31 ± 0.02	-2.26 ± 0.02	-0.80
111_trifluoropropan_2_ol	-6.05 ± 0.02	2.49 ± 0.02	-3.56 ± 0.03	-4.16
111_trimethoxyethane	-5.55 ± 0.01	1.66 ± 0.02	-3.89 ± 0.02	-4.42
1122_tetrachloroethane	-1.88 ± 0.03	1.47 ± 0.02	-0.41 ± 0.04	-2.47
112_trichloro_122_trifluoroethane	-0.32 ± 0.00	1.85 ± 0.02	1.53 ± 0.02	1.77
112_trichloroethane	-2.01 ± 0.02	1.51 ± 0.02	-0.50 ± 0.03	-1.99
11_diacetoxyethane	-9.52 ± 0.09	1.62 ± 0.03	-7.90 ± 0.10	-4.97
11_dichloroethane	-1.64 ± 0.01	1.81 ± 0.02	0.17 ± 0.02	-0.84
11_dichloroethene	-0.85 ± 0.00	2.09 ± 0.02	1.24 ± 0.02	0.25
11_diethoxyethane	-4.57 ± 0.01	2.39 ± 0.02	-2.18 ± 0.02	-3.28
11_difluoroethane	-2.41 ± 0.01	2.60 ± 0.02	0.19 ± 0.02	-0.11
1234_tetrachlorobenzene	-1.25 ± 0.01	0.93 ± 0.02	-0.32 ± 0.02	-1.34
1235_tetrachlorobenzene	-0.92 ± 0.00	0.90 ± 0.02	-0.02 ± 0.02	-1.62
123_trichlorobenzene	-1.67 ± 0.01	1.29 ± 0.02	-0.38 ± 0.02	-1.24
123_trimethylbenzene	-2.79 ± 0.01	2.14 ± 0.02	-0.65 ± 0.02	-1.21
1245_tetrachlorobenzene	-0.97 ± 0.00	1.22 ± 0.02	0.25 ± 0.02	-1.34
124_trichlorobenzene	-1.35 ± 0.00	1.17 ± 0.02	-0.18 ± 0.02	-1.12
124_trimethylbenzene	-2.75 ± 0.01	2.39 ± 0.02	-0.36 ± 0.02	-0.86
12_diacetoxyethane	-9.93 ± 0.02	1.61 ± 0.03	-8.32 ± 0.04	-6.34
12_dibromoethane	-1.60 ± 0.01	1.79 ± 0.02	0.19 ± 0.02	-2.33
12_dichlorobenzene	-1.96 ± 0.01	1.32 ± 0.02	-0.64 ± 0.02	-1.36
12_dichloroethane	-2.15 ± 0.01	1.63 ± 0.02	-0.52 ± 0.02	-1.79
12_dichloropropane	-2.13 ± 0.01	1.93 ± 0.02	-0.20 ± 0.02	-1.27
12_diethoxyethane	-5.47 ± 0.01	2.39 ± 0.03	-3.08 ± 0.03	-3.54
12_dimethoxyethane	-5.29 ± 0.01	1.93 ± 0.02	-3.36 ± 0.02	-4.84
12_ethanediol	-8.71 ± 0.02	1.09 ± 0.02	-7.62 ± 0.03	-9.30
135_trichlorobenzene	-0.96 ± 0.00	1.41 ± 0.02	0.45 ± 0.02	-0.78
135_trimethylbenzene	-2.73 ± 0.01	2.77 ± 0.02	0.04 ± 0.02	-0.90
13_dichlorobenzene	-1.60 ± 0.01	1.61 ± 0.02	0.01 ± 0.02	-0.98
13_dichloropropane	-2.18 ± 0.01	1.80 ± 0.02	-0.38 ± 0.02	-1.89
13_dimethylnaphthalene	-4.50 ± 0.01	1.71 ± 0.03	-2.79 ± 0.03	-2.47
14_dichlorobenzene	-1.63 ± 0.01	1.53 ± 0.02	-0.10 ± 0.02	-1.01
14_dichlorobutane	-2.38 ± 0.01	2.11 ± 0.02	-0.27 ± 0.02	-2.32
14_dimethyl_piperazine	-8.20 ± 0.02	0.80 ± 0.02	-7.40 ± 0.03	-7.58
14_dimethylnaphthalene	-4.50 ± 0.01	1.21 ± 0.03	-3.29 ± 0.03	-2.82
14_dioxane	-4.71 ± 0.01	0.36 ± 0.02	-4.35 ± 0.02	-5.06
1_bromo_2_chloroethane	-1.77 ± 0.01	1.79 ± 0.02	0.02 ± 0.02	-1.95
1_bromo_2_methylpropane	-0.95 ± 0.01	2.19 ± 0.02	1.24 ± 0.02	-0.03
1_bromobutane	-0.97 ± 0.00	2.65 ± 0.02	1.68 ± 0.02	-0.40
1_bromoheptane	-0.97 ± 0.00	2.63 ± 0.03	1.66 ± 0.03	0.34
1_bromohexane	-0.97 ± 0.00	2.75 ± 0.02	1.78 ± 0.02	0.18

1_bromooctane	-0.97 ± 0.00	2.89 ± 0.03	1.92 ± 0.03	0.52
1_bromopentane	-0.96 ± 0.00	2.44 ± 0.02	1.48 ± 0.02	-0.10
1_bromopropane	-0.98 ± 0.00	2.27 ± 0.02	1.29 ± 0.02	-0.56
1_chloro_222_trifluoroethane	-2.27 ± 0.01	2.43 ± 0.02	0.16 ± 0.02	0.06
1_chlorobutane	-1.22 ± 0.01	2.21 ± 0.02	0.99 ± 0.02	-0.16
1_chloroheptane	-1.21 ± 0.00	2.74 ± 0.03	1.53 ± 0.03	0.29
1_chlorohexane	-1.23 ± 0.01	2.46 ± 0.03	1.23 ± 0.03	0.00
1_chloropentane	-1.22 ± 0.01	2.40 ± 0.02	1.18 ± 0.02	-0.07
1_chloropropane	-1.25 ± 0.00	2.17 ± 0.02	0.92 ± 0.02	-0.33
1_ethylnaphthalene	-4.61 ± 0.01	1.61 ± 0.03	-3.00 ± 0.03	-2.40
1_iodobutane	-1.83 ± 0.01	2.41 ± 0.02	0.58 ± 0.02	-0.25
1_iodoheptane	-1.80 ± 0.01	2.99 ± 0.03	1.19 ± 0.03	0.27
1_iodohexane	-1.81 ± 0.01	2.47 ± 0.02	0.66 ± 0.02	0.08
1_iodopentane	-1.82 ± 0.01	2.48 ± 0.02	0.66 ± 0.02	-0.14
1_iodopropane	-1.87 ± 0.01	1.87 ± 0.02	0.00 ± 0.02	-0.53
1_methyl_imidazole	-7.06 ± 0.02	0.73 ± 0.02	-6.33 ± 0.03	-8.41
1_methyl_pyrrole	-3.90 ± 0.01	1.31 ± 0.02	-2.59 ± 0.02	-2.89
1_methylcyclohexene	-0.66 ± 0.00	1.99 ± 0.02	1.33 ± 0.02	0.67
1_methylnaphthalene	-4.52 ± 0.01	1.28 ± 0.02	-3.24 ± 0.02	-2.44
1_naphthol	-8.31 ± 0.02	0.80 ± 0.02	-7.51 ± 0.03	-7.67
1_naphthylamine	-8.63 ± 0.02	0.87 ± 0.02	-7.76 ± 0.03	-7.28
1_nitrobutane	-2.43 ± 0.01	0.92 ± 0.02	-1.51 ± 0.02	-3.09
1_nitropentane	-2.40 ± 0.01	1.11 ± 0.02	-1.29 ± 0.02	-2.82
1_nitropropane	-2.44 ± 0.01	1.06 ± 0.02	-1.38 ± 0.02	-3.34
222_trifluoroethanol	-6.05 ± 0.02	2.10 ± 0.02	-3.95 ± 0.03	-4.31
224_trimethylpentane	0.02 ± 0.00	2.91 ± 0.03	2.93 ± 0.03	2.89
225_trimethylhexane	0.00 ± 0.00	2.86 ± 0.03	2.86 ± 0.03	2.93
22_dimethylbutane	0.01 ± 0.00	2.52 ± 0.02	2.53 ± 0.02	2.51
22_dimethylpentane	0.01 ± 0.00	2.89 ± 0.02	2.90 ± 0.02	2.88
22_dimethylpropane	0.01 ± 0.00	2.59 ± 0.02	2.60 ± 0.02	2.51
234_trimethylpentane	0.01 ± 0.00	2.85 ± 0.03	2.86 ± 0.03	2.56
23_dimethylbuta_13_diene	-1.11 ± 0.01	2.80 ± 0.02	1.69 ± 0.02	0.40
23_dimethylbutane	0.01 ± 0.00	2.68 ± 0.02	2.69 ± 0.02	2.34
23_dimethylnaphthalene	-4.43 ± 0.01	1.84 ± 0.02	-2.59 ± 0.02	-2.78
23_dimethylpentane	0.00 ± 0.00	2.66 ± 0.03	2.66 ± 0.03	2.52
23_dimethylphenol	-6.49 ± 0.02	1.82 ± 0.02	-4.67 ± 0.03	-6.16
23_dimethylpyridine	-4.79 ± 0.01	1.52 ± 0.02	-3.27 ± 0.02	-4.82
24_dimethylpentan_3_one	-5.13 ± 0.01	2.66 ± 0.02	-2.47 ± 0.02	-2.74
24_dimethylpentane	0.00 ± 0.00	2.89 ± 0.03	2.89 ± 0.03	2.83
24_dimethylphenol	-6.48 ± 0.02	1.93 ± 0.02	-4.55 ± 0.03	-6.01
24_dimethylpyridine	-4.94 ± 0.01	1.76 ± 0.02	-3.18 ± 0.02	-4.86
25_dimethylphenol	-5.97 ± 0.02	1.58 ± 0.02	-4.39 ± 0.03	-5.91
25_dimethylpyridine	-4.76 ± 0.01	1.93 ± 0.02	-2.83 ± 0.02	-4.72
25_dimethyltetrahydrofuran	-3.52 ± 0.01	1.63 ± 0.02	-1.89 ± 0.02	-2.92
26_dimethylaniline	-6.51 ± 0.02	1.64 ± 0.02	-4.87 ± 0.03	-5.21
26_dimethylnaphthalene	-4.42 ± 0.01	1.77 ± 0.03	-2.65 ± 0.03	-2.63
26_dimethylphenol	-5.78 ± 0.02	1.69 ± 0.02	-4.09 ± 0.03	-5.26
26_dimethylpyridine	-5.15 ± 0.01	1.79 ± 0.02	-3.36 ± 0.02	-4.59
2_bromo_2_methylpropane	-1.25 ± 0.01	2.14 ± 0.02	0.89 ± 0.02	0.84
2_bromopropane	-1.16 ± 0.01	2.13 ± 0.02	0.97 ± 0.02	-0.48
2_butoxyethanol	-5.94 ± 0.02	1.87 ± 0.02	-4.07 ± 0.03	-6.25
2_chloro_111_trimethoxyethane	-5.40 ± 0.02	2.10 ± 0.03	-3.30 ± 0.04	-4.59
2_chloro_2_methylpropane	-1.44 ± 0.01	2.26 ± 0.02	0.82 ± 0.02	1.09
2_chloroaniline	-6.04 ± 0.02	1.08 ± 0.02	-4.96 ± 0.03	-4.91
2_chlorobutane	-1.35 ± 0.00	2.56 ± 0.02	1.21 ± 0.02	0.00
2_chlorophenol	-4.51 ± 0.02	1.28 ± 0.02	-3.23 ± 0.03	-4.55
2_chloropropane	-1.40 ± 0.01	2.22 ± 0.02	0.82 ± 0.02	-0.25
2_chloropyridine	-4.85 ± 0.01	1.49 ± 0.02	-3.36 ± 0.02	-4.39
2_chlorotoluene	-2.18 ± 0.01	1.67 ± 0.02	-0.51 ± 0.02	-1.14
2_ethoxyethanol	-6.41 ± 0.02	1.64 ± 0.02	-4.77 ± 0.03	-6.69
2_ethylpyrazine	-6.94 ± 0.02	1.26 ± 0.02	-5.68 ± 0.03	-5.45

2_ethylpyridine	-4.96 ± 0.01	1.75 ± 0.02	-3.21 ± 0.02	-4.33
2_ethyltoluene	-2.85 ± 0.01	2.19 ± 0.03	-0.66 ± 0.03	-1.04
2_fluorophenol	-4.89 ± 0.03	1.65 ± 0.02	-3.24 ± 0.03	-5.29
2_iodophenol	-3.93 ± 0.03	1.02 ± 0.02	-2.91 ± 0.03	-6.20
2_iodopropane	-1.97 ± 0.01	2.26 ± 0.02	0.29 ± 0.02	-0.46
2_isobutylpyrazine	-6.81 ± 0.01	1.71 ± 0.03	-5.10 ± 0.03	-5.04
2_methoxy_111_trimethoxyethane	-7.61 ± 0.02	1.64 ± 0.03	-5.97 ± 0.04	-5.73
2_methoxyaniline	-7.69 ± 0.02	1.16 ± 0.02	-6.53 ± 0.03	-6.12
2_methoxyethanamine	-7.04 ± 0.02	1.42 ± 0.02	-5.62 ± 0.03	-6.55
2_methoxyethanol	-6.92 ± 0.02	1.55 ± 0.02	-5.37 ± 0.03	-6.76
2_methoxyphenol	-6.00 ± 0.02	1.26 ± 0.02	-4.74 ± 0.03	-5.57
2_methyl_but_2_ene	-0.56 ± 0.00	2.94 ± 0.02	2.38 ± 0.02	1.31
2_methylbut_2_ene	-0.55 ± 0.00	2.83 ± 0.02	2.28 ± 0.02	1.31
2_methylbuta_13_diene	-1.12 ± 0.01	2.93 ± 0.02	1.81 ± 0.02	0.68
2_methylbutan_1_ol	-4.88 ± 0.01	2.10 ± 0.02	-2.78 ± 0.02	-4.42
2_methylbutan_2_ol	-5.17 ± 0.02	2.21 ± 0.02	-2.96 ± 0.03	-4.43
2_methylbutane	0.01 ± 0.00	2.51 ± 0.02	2.52 ± 0.02	2.38
2_methylhexane	0.01 ± 0.00	2.99 ± 0.03	3.00 ± 0.03	2.93
2_methylpent_1_ene	-0.40 ± 0.00	3.15 ± 0.02	2.75 ± 0.02	1.47
2_methylpentan_2_ol	-5.13 ± 0.01	2.34 ± 0.02	-2.79 ± 0.02	-3.92
2_methylpentan_3_ol	-4.75 ± 0.02	2.56 ± 0.02	-2.19 ± 0.03	-3.88
2_methylpentane	0.01 ± 0.00	2.77 ± 0.02	2.78 ± 0.02	2.51
2_methylpropan_1_ol	-5.02 ± 0.01	2.06 ± 0.02	-2.96 ± 0.02	-4.50
2_methylpropan_2_ol	-5.31 ± 0.01	2.22 ± 0.02	-3.09 ± 0.02	-4.47
2_methylpropane	0.01 ± 0.00	2.73 ± 0.02	2.74 ± 0.02	2.32
2_methylpropene	-0.45 ± 0.00	2.79 ± 0.02	2.34 ± 0.02	1.16
2_methylpyrazine	-6.99 ± 0.02	0.89 ± 0.02	-6.10 ± 0.03	-5.51
2_methylpyridine	-4.95 ± 0.01	1.54 ± 0.02	-3.41 ± 0.02	-4.63
2_methyltetrahydrofuran	-3.39 ± 0.01	1.44 ± 0.02	-1.95 ± 0.02	-3.30
2_methylthiophene	-1.90 ± 0.01	1.68 ± 0.02	-0.22 ± 0.02	-1.38
2_naphthol	-8.70 ± 0.02	0.82 ± 0.02	-7.88 ± 0.03	-8.11
2_naphthylamine	-8.83 ± 0.02	0.96 ± 0.02	-7.87 ± 0.03	-7.47
2_nitroaniline	-7.84 ± 0.02	-0.12 ± 0.02	-7.96 ± 0.03	-7.37
2_nitrophenol	-5.40 ± 0.02	0.06 ± 0.02	-5.34 ± 0.03	-4.58
2_nitropropane	-2.54 ± 0.01	0.93 ± 0.02	-1.61 ± 0.02	-3.13
2_nitrotoluene	-3.79 ± 0.01	0.65 ± 0.02	-3.14 ± 0.02	-3.58
2_phenylethanol	-7.05 ± 0.02	1.72 ± 0.02	-5.33 ± 0.03	-6.79
2_propoxyethanol	-6.14 ± 0.02	1.93 ± 0.02	-4.21 ± 0.03	-6.40
333_trimethoxypropionitrile	-6.88 ± 0.02	1.95 ± 0.03	-4.93 ± 0.04	-6.40
33_dimethylbutan_2_one	-5.18 ± 0.01	2.27 ± 0.02	-2.91 ± 0.02	-3.11
33_dimethylpentane	0.01 ± 0.00	2.52 ± 0.03	2.53 ± 0.03	2.56
34_dimethylphenol	-6.86 ± 0.02	1.53 ± 0.02	-5.33 ± 0.03	-6.50
34_dimethylpyridine	-4.59 ± 0.01	1.41 ± 0.02	-3.18 ± 0.02	-5.22
35_dimethylphenol	-7.01 ± 0.02	1.89 ± 0.02	-5.12 ± 0.03	-6.27
35_dimethylpyridine	-4.47 ± 0.01	1.53 ± 0.02	-2.94 ± 0.02	-4.84
3_acetylpyridine	-8.04 ± 0.02	0.94 ± 0.02	-7.10 ± 0.03	-8.26
3_chloroaniline	-6.41 ± 0.01	1.04 ± 0.02	-5.37 ± 0.02	-5.82
3_chlorophenol	-6.38 ± 0.02	1.10 ± 0.02	-5.28 ± 0.03	-6.62
3_chloroprop_1_ene	-1.48 ± 0.01	2.36 ± 0.02	0.88 ± 0.02	-0.57
3_chloropyridine	-3.78 ± 0.01	1.28 ± 0.02	-2.50 ± 0.02	-4.01
3_cyanophenol	-8.16 ± 0.02	1.12 ± 0.02	-7.04 ± 0.03	-9.65
3_cyanopyridine	-5.79 ± 0.01	1.13 ± 0.02	-4.66 ± 0.02	-6.75
3_ethylphenol	-6.91 ± 0.02	1.89 ± 0.02	-5.02 ± 0.03	-6.25
3_ethylpyridine	-4.59 ± 0.01	1.63 ± 0.02	-2.96 ± 0.02	-4.59
3_formylpyridine	-8.22 ± 0.02	0.58 ± 0.02	-7.64 ± 0.03	-7.10
3_hydroxybenzaldehyde	-10.18 ± 0.02	0.94 ± 0.02	-9.24 ± 0.03	-9.50
3_methoxyaniline	-8.44 ± 0.02	0.99 ± 0.02	-7.45 ± 0.03	-7.29
3_methoxyphenol	-8.10 ± 0.02	1.07 ± 0.02	-7.03 ± 0.03	-7.66
3_methyl_1h_indole	-7.53 ± 0.02	0.98 ± 0.02	-6.55 ± 0.03	-5.88
3_methyl_but_1_ene	-0.33 ± 0.00	3.13 ± 0.02	2.80 ± 0.02	1.83
3_methylbut_1_ene	-0.34 ± 0.00	3.01 ± 0.02	2.67 ± 0.02	1.82

3_methylbutan_1_ol	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-4.42
3_methylbutan_2_one	-5.34 ± 0.01	2.41 ± 0.02	-2.93 ± 0.02	-3.24
3_methylbutanoic_acid	-6.99 ± 0.02	1.48 ± 0.02	-5.51 ± 0.03	-6.09
3_methylheptane	0.01 ± 0.00	3.28 ± 0.03	3.29 ± 0.03	2.97
3_methylhexane	0.00 ± 0.00	2.76 ± 0.02	2.76 ± 0.02	2.71
3_methylpentane	0.00 ± 0.00	2.72 ± 0.02	2.72 ± 0.02	2.51
3_methylpyridine	-4.56 ± 0.01	1.37 ± 0.02	-3.19 ± 0.02	-4.77
3_nitroaniline	-8.00 ± 0.02	-0.24 ± 0.02	-8.24 ± 0.03	-8.84
3_nitrophenol	-7.45 ± 0.02	-0.21 ± 0.02	-7.66 ± 0.03	-9.62
3_nitrotoluene	-3.51 ± 0.01	0.35 ± 0.02	-3.16 ± 0.02	-3.45
3_phenylpropanol	-7.38 ± 0.03	1.88 ± 0.02	-5.50 ± 0.03	-6.92
4_acetylpyridine	-8.38 ± 0.02	0.75 ± 0.02	-7.63 ± 0.03	-7.62
4_bromophenol	-6.59 ± 0.01	1.12 ± 0.02	-5.47 ± 0.02	-7.13
4_bromotoluene	-2.20 ± 0.01	2.24 ± 0.02	0.04 ± 0.02	-1.39
4_chloro_3_methylphenol	-6.38 ± 0.02	1.48 ± 0.02	-4.90 ± 0.03	-6.79
4_chloroaniline	-6.47 ± 0.01	1.19 ± 0.02	-5.28 ± 0.02	-5.90
4_chlorophenol	-6.53 ± 0.01	1.17 ± 0.02	-5.36 ± 0.02	-7.03
4_cyanophenol	-8.72 ± 0.02	1.11 ± 0.02	-7.61 ± 0.03	-10.17
4_cyanopyridine	-5.99 ± 0.01	1.02 ± 0.02	-4.97 ± 0.02	-6.02
4_ethylphenol	-7.07 ± 0.02	1.99 ± 0.02	-5.08 ± 0.03	-6.13
4_ethylpyridine	-4.72 ± 0.01	1.85 ± 0.02	-2.87 ± 0.02	-4.73
4_ethyltoluene	-2.78 ± 0.01	2.73 ± 0.02	-0.05 ± 0.02	-0.95
4_fluorophenol	-6.51 ± 0.02	1.52 ± 0.02	-4.99 ± 0.03	-6.19
4_formylpyridine	-8.13 ± 0.02	0.82 ± 0.02	-7.31 ± 0.03	-7.00
4_hydroxybenzaldehyde	-10.85 ± 0.02	0.85 ± 0.02	-10.00 ± 0.03	-8.83
4_isopropyltoluene	-2.53 ± 0.01	2.73 ± 0.03	0.20 ± 0.03	-0.68
4_methoxyacetophenone	-7.89 ± 0.01	1.60 ± 0.03	-6.29 ± 0.03	-4.40
4_methoxyaniline	-8.09 ± 0.02	1.17 ± 0.02	-6.92 ± 0.03	-7.48
4_methyl_1h_imidazole	-8.85 ± 0.02	0.86 ± 0.02	-7.99 ± 0.03	-10.27
4_methylacetophenone	-6.70 ± 0.02	1.88 ± 0.02	-4.82 ± 0.03	-4.70
4_methylbenzaldehyde	-6.43 ± 0.02	1.53 ± 0.02	-4.90 ± 0.03	-4.27
4_methylpentan_2_ol	-5.10 ± 0.01	2.35 ± 0.02	-2.75 ± 0.02	-3.73
4_methylpentan_2_one	-5.28 ± 0.01	2.32 ± 0.02	-2.96 ± 0.02	-3.05
4_methylpyridine	-4.73 ± 0.01	1.32 ± 0.02	-3.41 ± 0.02	-4.93
4_n_propylphenol	-6.96 ± 0.01	1.46 ± 0.02	-5.50 ± 0.02	-5.90
4_nitroaniline	-9.03 ± 0.02	-0.20 ± 0.02	-9.23 ± 0.03	-10.27
4_nitrophenol	-8.04 ± 0.01	-0.18 ± 0.02	-8.22 ± 0.02	-10.64
4_tert_butylphenol	-7.21 ± 0.02	1.67 ± 0.03	-5.54 ± 0.04	-5.91
E_12_dichloroethene	-0.87 ± 0.00	2.07 ± 0.02	1.20 ± 0.02	-0.78
E_but_2_enal	-5.82 ± 0.01	2.16 ± 0.02	-3.66 ± 0.02	-4.22
E_hept_2_ene	-0.43 ± 0.00	3.26 ± 0.02	2.83 ± 0.02	1.68
E_hex_2_enal	-5.48 ± 0.01	2.26 ± 0.02	-3.22 ± 0.02	-3.68
E_oct_2_enal	-5.37 ± 0.01	2.90 ± 0.03	-2.47 ± 0.03	-3.43
NN_dimethyl_p_methoxybenzamide	-10.16 ± 0.02	0.87 ± 0.04	-9.29 ± 0.04	-11.01
NN_dimethyl_p_methylbenzamide	-9.10 ± 0.02	1.59 ± 0.04	-7.51 ± 0.04	-9.76
NN_dimethyl_p_nitrobenzamide	-9.24 ± 0.02	-0.68 ± 0.03	-9.92 ± 0.04	-11.95
NN_dimethylaniline	-6.13 ± 0.01	1.43 ± 0.02	-4.70 ± 0.02	-3.45
NN_dimethylbenzamide	-9.17 ± 0.02	1.19 ± 0.03	-7.98 ± 0.04	-9.29
NN_dimethylformamide	-8.13 ± 0.02	1.27 ± 0.02	-6.86 ± 0.03	-7.81
N_acetylpyrrolidine	-8.86 ± 0.01	0.89 ± 0.02	-7.97 ± 0.02	-9.80
N_methyl_N__222_trifluoroethyl__aniline	-6.24 ± 0.01	2.55 ± 0.03	-3.69 ± 0.03	-1.92
N_methylacetamide	-9.93 ± 0.02	1.54 ± 0.02	-8.39 ± 0.03	-10.00
N_methylaniline	-7.10 ± 0.02	1.36 ± 0.02	-5.74 ± 0.03	-4.69
N_methylmorpholine	-6.46 ± 0.02	0.59 ± 0.02	-5.87 ± 0.03	-6.32
N_methylpiperazine	-8.40 ± 0.02	0.10 ± 0.02	-8.30 ± 0.03	-7.77
N_methylpiperidine	-4.18 ± 0.01	0.97 ± 0.02	-3.21 ± 0.02	-3.88
Z_12_dichloroethene	-1.72 ± 0.01	2.03 ± 0.02	0.31 ± 0.02	-1.17
Z_pent_2_ene	-0.42 ± 0.00	2.97 ± 0.02	2.55 ± 0.02	1.31
acenaphthene	-4.89 ± 0.01	1.38 ± 0.03	-3.51 ± 0.03	-3.15
acetaldehyde	-5.18 ± 0.01	1.79 ± 0.02	-3.39 ± 0.02	-3.50
acetic_acid	-7.07 ± 0.02	1.12 ± 0.01	-5.95 ± 0.02	-6.69

acetonitrile	-3.77 ± 0.01	2.10 ± 0.01	-1.67 ± 0.01	-3.88
acetophenone	-6.67 ± 0.02	1.60 ± 0.02	-5.07 ± 0.03	-4.58
alpha_methylstyrene	-3.53 ± 0.01	2.27 ± 0.02	-1.26 ± 0.02	-1.24
ammonia	-5.82 ± 0.01	1.78 ± 0.01	-4.04 ± 0.01	-4.29
aniline	-7.00 ± 0.01	1.08 ± 0.02	-5.92 ± 0.02	-5.49
anisole	-3.98 ± 0.01	1.68 ± 0.02	-2.30 ± 0.02	-2.45
anthracene	-5.97 ± 0.01	0.58 ± 0.03	-5.39 ± 0.03	-3.95
azetidine	-5.09 ± 0.01	1.68 ± 0.02	-3.41 ± 0.02	-5.56
benzaldehyde	-6.36 ± 0.01	1.37 ± 0.02	-4.99 ± 0.02	-4.02
benzamide	-10.97 ± 0.02	0.78 ± 0.02	-10.19 ± 0.03	-11.00
benzene	-2.70 ± 0.01	2.00 ± 0.02	-0.70 ± 0.02	-0.86
benzonitrile	-4.13 ± 0.01	1.39 ± 0.02	-2.74 ± 0.02	-4.21
benzotrifluoride	-3.02 ± 0.01	2.47 ± 0.02	-0.55 ± 0.02	-0.25
benzyl_alcohol	-6.94 ± 0.02	1.53 ± 0.02	-5.41 ± 0.03	-6.62
benzyl_bromide	-3.13 ± 0.01	1.99 ± 0.02	-1.14 ± 0.02	-2.38
benzyl_chloride	-3.37 ± 0.01	1.81 ± 0.02	-1.56 ± 0.02	-1.93
biphenyl	-4.97 ± 0.01	1.58 ± 0.02	-3.39 ± 0.02	-2.66
bis_2_chloroethyl__ether	-3.78 ± 0.01	1.92 ± 0.02	-1.86 ± 0.02	-4.23
bromobenzene	-2.20 ± 0.01	1.83 ± 0.02	-0.37 ± 0.02	-1.46
bromoethane	-1.01 ± 0.01	1.94 ± 0.02	0.93 ± 0.02	-0.74
bromomethane	-0.89 ± 0.00	1.98 ± 0.01	1.09 ± 0.01	-0.82
bromotrifluoromethane	-0.38 ± 0.00	2.41 ± 0.02	2.03 ± 0.02	1.79
but_1_ene	-0.37 ± 0.00	2.85 ± 0.02	2.48 ± 0.02	1.38
but_1_yne	-0.86 ± 0.00	2.79 ± 0.02	1.93 ± 0.02	-0.16
buta_13_diene	-0.96 ± 0.01	2.89 ± 0.02	1.93 ± 0.02	0.61
butan_1_ol	-5.12 ± 0.01	1.98 ± 0.02	-3.14 ± 0.02	-4.72
butan_2_ol	-5.20 ± 0.02	2.08 ± 0.02	-3.12 ± 0.03	-4.62
butanenitrile	-3.57 ± 0.01	2.16 ± 0.02	-1.41 ± 0.02	-3.64
butanoic_acid	-6.92 ± 0.02	1.46 ± 0.02	-5.46 ± 0.03	-6.35
butanone	-5.05 ± 0.01	2.08 ± 0.02	-2.97 ± 0.02	-3.71
butyraldehyde	-5.07 ± 0.01	2.06 ± 0.02	-3.01 ± 0.02	-3.18
chlorobenzene	-2.13 ± 0.01	1.53 ± 0.02	-0.60 ± 0.02	-1.12
chlorodifluoromethane	-2.32 ± 0.01	2.28 ± 0.02	-0.04 ± 0.02	-0.50
chloroethane	-1.26 ± 0.01	2.04 ± 0.02	0.78 ± 0.02	-0.63
chloroethylene	-1.06 ± 0.00	2.28 ± 0.02	1.22 ± 0.02	-0.59
chlorofluoromethane	-2.25 ± 0.01	2.03 ± 0.01	-0.22 ± 0.01	-0.77
chloromethane	-1.14 ± 0.01	1.95 ± 0.01	0.81 ± 0.01	-0.55
cis_12_dimethylcyclohexane	0.02 ± 0.00	2.03 ± 0.02	2.05 ± 0.02	1.58
cyanobenzene	-4.14 ± 0.01	1.76 ± 0.02	-2.38 ± 0.02	-4.10
cyclohepta_135_triene	-1.97 ± 0.01	2.12 ± 0.02	0.15 ± 0.02	-0.99
cycloheptanol	-5.14 ± 0.01	0.99 ± 0.05	-4.15 ± 0.05	-5.48
cyclohexane	0.01 ± 0.00	1.66 ± 0.02	1.67 ± 0.02	1.23
cyclohexanol	-5.28 ± 0.01	1.02 ± 0.02	-4.26 ± 0.02	-5.46
cyclohexanone	-5.14 ± 0.01	1.30 ± 0.02	-3.84 ± 0.02	-4.91
cyclohexene	-0.53 ± 0.00	2.09 ± 0.02	1.56 ± 0.02	0.37
cyclohexylamine	-5.08 ± 0.01	1.14 ± 0.02	-3.94 ± 0.02	-4.59
cyclopentane	0.01 ± 0.00	1.52 ± 0.02	1.53 ± 0.02	1.20
cyclopentanol	-5.27 ± 0.01	1.12 ± 0.02	-4.15 ± 0.02	-5.49
cyclopentanone	-4.85 ± 0.01	1.14 ± 0.02	-3.71 ± 0.02	-4.70
cyclopentene	-0.58 ± 0.00	1.96 ± 0.02	1.38 ± 0.02	0.56
cyclopropane	-0.03 ± 0.00	2.67 ± 0.02	2.64 ± 0.02	0.75
decan_1_ol	-5.16 ± 0.01	2.67 ± 0.03	-2.49 ± 0.03	-3.64
decan_2_one	-5.26 ± 0.01	3.28 ± 0.03	-1.98 ± 0.03	-2.34
di_isopropyl_sulfide	-2.56 ± 0.01	2.66 ± 0.02	0.10 ± 0.02	-1.21
di_n_butyl_ether	-2.65 ± 0.01	3.24 ± 0.03	0.59 ± 0.03	-0.83
di_n_butylamine	-4.71 ± 0.01	3.08 ± 0.03	-1.63 ± 0.03	-3.24
di_n_propyl_ether	-2.67 ± 0.01	2.88 ± 0.02	0.21 ± 0.02	-1.16
di_n_propyl_sulfide	-2.15 ± 0.01	2.64 ± 0.02	0.49 ± 0.02	-1.28
di_n_propylamine	-4.76 ± 0.01	2.50 ± 0.02	-2.26 ± 0.02	-3.65
dibromomethane	-1.10 ± 0.00	1.97 ± 0.02	0.87 ± 0.02	-1.96
dichloromethane	-1.60 ± 0.01	1.83 ± 0.01	0.23 ± 0.01	-1.31

diethoxymethoxybenzene	-7.19 ± 0.02	2.75 ± 0.03	-4.44 ± 0.04	-5.23
diethyl_disulfide	-2.51 ± 0.01	2.44 ± 0.02	-0.07 ± 0.02	-1.64
diethyl_ether	-3.02 ± 0.01	2.32 ± 0.02	-0.70 ± 0.02	-1.59
diethyl_malonate	-8.27 ± 0.02	1.82 ± 0.03	-6.45 ± 0.04	-6.00
diethyl_succinate	-10.32 ± 0.02	1.85 ± 0.03	-8.47 ± 0.04	-5.71
diethyl_sulfide	-2.18 ± 0.01	2.39 ± 0.02	0.21 ± 0.02	-1.46
diethylamine	-4.93 ± 0.01	2.21 ± 0.02	-2.72 ± 0.02	-4.07
diiodomethane	-2.30 ± 0.01	1.56 ± 0.02	-0.74 ± 0.02	-2.49
diisopropyl_ether	-3.01 ± 0.01	2.90 ± 0.02	-0.11 ± 0.02	-0.53
diisopropylamine	-4.60 ± 0.01	2.63 ± 0.02	-1.97 ± 0.02	-3.22
dimethoxymethane	-4.33 ± 0.01	1.64 ± 0.02	-2.69 ± 0.02	-2.93
dimethyl_disulfide	-0.72 ± 0.00	2.20 ± 0.02	1.48 ± 0.02	-1.83
dimethyl_ether	-2.70 ± 0.01	1.85 ± 0.02	-0.85 ± 0.02	-1.91
dimethyl_sulfate	-8.13 ± 0.01	0.28 ± 0.02	-7.85 ± 0.02	-5.10
dimethyl_sulfide	-1.70 ± 0.01	1.96 ± 0.02	0.26 ± 0.02	-1.61
dimethyl_sulfone	-11.21 ± 0.02	0.85 ± 0.02	-10.36 ± 0.03	-10.08
dimethyl_sulfoxide	-9.68 ± 0.02	1.36 ± 0.02	-8.32 ± 0.03	-8.71
dimethylamine	-4.72 ± 0.01	1.61 ± 0.02	-3.11 ± 0.02	-4.29
ethanamide	-9.94 ± 0.02	1.32 ± 0.02	-8.62 ± 0.03	-9.71
ethane	0.00 ± 0.00	2.58 ± 0.01	2.58 ± 0.01	1.83
ethanethiol	-2.49 ± 0.01	2.09 ± 0.02	-0.40 ± 0.02	-1.14
ethanol	-5.20 ± 0.02	1.75 ± 0.02	-3.45 ± 0.03	-5.00
ethene	-0.30 ± 0.00	2.66 ± 0.01	2.36 ± 0.01	1.28
ethyl_acetate	-5.14 ± 0.01	1.91 ± 0.02	-3.23 ± 0.02	-2.94
ethyl_benzoate	-6.33 ± 0.01	1.65 ± 0.02	-4.68 ± 0.02	-3.64
ethyl_butanoate	-5.39 ± 0.01	2.35 ± 0.02	-3.04 ± 0.02	-2.49
ethyl_formate	-4.52 ± 0.01	1.53 ± 0.02	-2.99 ± 0.02	-2.56
ethyl_hexanoate	-5.43 ± 0.02	2.63 ± 0.03	-2.80 ± 0.04	-2.23
ethyl_pentanoate	-5.47 ± 0.01	2.38 ± 0.03	-3.09 ± 0.03	-2.49
ethyl_phenyl_ether	-4.12 ± 0.01	2.11 ± 0.02	-2.01 ± 0.02	-2.22
ethyl_propanoate	-5.51 ± 0.01	2.12 ± 0.02	-3.39 ± 0.02	-2.68
ethylamine	-5.00 ± 0.01	1.86 ± 0.02	-3.14 ± 0.02	-4.50
ethylbenzene	-2.76 ± 0.01	2.17 ± 0.02	-0.59 ± 0.02	-0.79
fluorene	-5.31 ± 0.01	1.02 ± 0.02	-4.29 ± 0.02	-3.35
fluorobenzene	-2.10 ± 0.01	2.03 ± 0.02	-0.07 ± 0.02	-0.80
fluoromethane	-1.61 ± 0.01	2.40 ± 0.01	0.79 ± 0.01	-0.22
formaldehyde	-4.87 ± 0.01	1.65 ± 0.01	-3.22 ± 0.01	-2.75
halothane	-1.59 ± 0.01	2.29 ± 0.02	0.70 ± 0.02	-0.11
hept_1_ene	-0.33 ± 0.00	3.30 ± 0.02	2.97 ± 0.02	1.66
hept_1_yne	-0.80 ± 0.00	3.08 ± 0.02	2.28 ± 0.02	0.60
heptan_1_ol	-5.09 ± 0.01	2.37 ± 0.02	-2.72 ± 0.02	-4.21
heptan_2_one	-5.30 ± 0.01	2.50 ± 0.02	-2.80 ± 0.02	-3.04
heptan_4_one	-5.19 ± 0.01	2.51 ± 0.02	-2.68 ± 0.02	-2.92
heptanal	-5.06 ± 0.01	2.43 ± 0.03	-2.63 ± 0.03	-2.67
hex_1_ene	-0.33 ± 0.00	2.92 ± 0.02	2.59 ± 0.02	1.58
hex_1_yne	-0.81 ± 0.00	2.91 ± 0.02	2.10 ± 0.02	0.29
hexa_15_diene	-0.65 ± 0.01	3.09 ± 0.02	2.44 ± 0.02	1.01
hexafluoropropene	-1.17 ± 0.01	3.46 ± 0.02	2.29 ± 0.02	-3.76
hexan_1_ol	-5.08 ± 0.01	2.05 ± 0.02	-3.03 ± 0.02	-4.40
hexan_2_one	-5.28 ± 0.01	2.51 ± 0.02	-2.77 ± 0.02	-3.28
hexan_3_ol	-4.96 ± 0.01	2.33 ± 0.02	-2.63 ± 0.02	-4.06
hexanal	-5.09 ± 0.01	2.13 ± 0.02	-2.96 ± 0.02	-2.81
hexanoic_acid	-6.93 ± 0.02	1.85 ± 0.02	-5.08 ± 0.03	-6.21
hydrazine	-8.36 ± 0.02	1.26 ± 0.01	-7.10 ± 0.02	-9.30
hydrogen_sulfide	-3.05 ± 0.01	1.88 ± 0.01	-1.17 ± 0.01	-0.70
imidazole	-8.49 ± 0.02	0.64 ± 0.02	-7.85 ± 0.03	-9.63
indane	-2.97 ± 0.01	1.27 ± 0.02	-1.70 ± 0.02	-1.46
iodobenzene	-2.11 ± 0.01	1.77 ± 0.02	-0.34 ± 0.02	-1.74
iodoethane	-1.93 ± 0.01	1.83 ± 0.02	-0.10 ± 0.02	-0.74
iodomethane	-1.90 ± 0.01	1.93 ± 0.01	0.03 ± 0.01	-0.89
isoamyl_acetate	-5.44 ± 0.01	2.39 ± 0.03	-3.05 ± 0.03	-2.21

isoamyl_formate	-5.17 ± 0.01	1.78 ± 0.02	-3.39 ± 0.02	-2.13
isobutyl_acetate	-5.23 ± 0.01	2.43 ± 0.02	-2.80 ± 0.02	-2.36
isobutyl_formate	-5.00 ± 0.01	1.79 ± 0.02	-3.21 ± 0.02	-2.22
isobutyl_isobutanoate	-5.29 ± 0.01	2.74 ± 0.03	-2.55 ± 0.03	-1.69
isobutylbenzene	-2.66 ± 0.01	2.66 ± 0.02	0.00 ± 0.02	0.16
isobutyraldehyde	-4.98 ± 0.01	2.05 ± 0.02	-2.93 ± 0.02	-2.86
isoflurane	-4.21 ± 0.01	2.83 ± 0.02	-1.38 ± 0.02	0.10
isopropyl_acetate	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-2.64
isopropyl_formate	-4.37 ± 0.01	1.73 ± 0.02	-2.64 ± 0.02	-2.02
isopropylbenzene	-2.86 ± 0.01	2.55 ± 0.02	-0.31 ± 0.02	-0.30
m_bis_trifluoromethyl__benzene	-4.19 ± 0.01	2.61 ± 0.03	-1.58 ± 0.03	1.07
m_cresol	-6.94 ± 0.02	1.66 ± 0.02	-5.28 ± 0.03	-5.49
m_xylene	-2.71 ± 0.01	2.54 ± 0.02	-0.17 ± 0.02	-0.83
methane	0.00 ± 0.00	2.54 ± 0.01	2.54 ± 0.01	1.99
methanesulfonyl_chloride	-6.85 ± 0.01	0.52 ± 0.02	-6.33 ± 0.02	-4.87
methanethiol	-2.25 ± 0.01	1.99 ± 0.01	-0.26 ± 0.01	-1.24
methanol	-5.15 ± 0.01	1.67 ± 0.01	-3.48 ± 0.01	-5.10
methoxyflurane	-2.49 ± 0.01	1.78 ± 0.02	-0.71 ± 0.02	-1.12
methyl_acetate	-5.44 ± 0.01	1.71 ± 0.02	-3.73 ± 0.02	-3.13
methyl_benzoate	-6.30 ± 0.02	1.24 ± 0.02	-5.06 ± 0.03	-3.92
methyl_butanoate	-5.36 ± 0.01	2.04 ± 0.02	-3.32 ± 0.02	-2.83
methyl_chloroacetate	-5.16 ± 0.01	1.24 ± 0.02	-3.92 ± 0.02	-4.00
methyl_cyanoacetate	-6.89 ± 0.01	1.38 ± 0.02	-5.51 ± 0.02	-6.72
methyl_cyclohexanecarboxylate	-5.51 ± 0.01	1.22 ± 0.02	-4.29 ± 0.02	-3.30
methyl_cyclohexyl_ketone	-5.38 ± 0.01	1.48 ± 0.02	-3.90 ± 0.02	-3.90
methyl_cyclopropanecarboxylate	-6.30 ± 0.02	1.81 ± 0.03	-4.49 ± 0.04	-4.10
methyl_cyclopropyl_ketone	-5.82 ± 0.01	2.08 ± 0.02	-3.74 ± 0.02	-4.61
methyl_ethyl_ether	-2.84 ± 0.01	2.02 ± 0.02	-0.82 ± 0.02	-2.10
methyl_ethyl_sulfide	-1.93 ± 0.01	2.27 ± 0.02	0.34 ± 0.02	-1.50
methyl_formate	-4.48 ± 0.01	1.31 ± 0.02	-3.17 ± 0.02	-2.78
methyl_hexanoate	-5.36 ± 0.01	2.34 ± 0.03	-3.02 ± 0.03	-2.49
methyl_isopropyl_ether	-2.89 ± 0.01	2.14 ± 0.02	-0.75 ± 0.02	-2.01
methyl_methanesulfonate	-8.81 ± 0.02	0.52 ± 0.02	-8.29 ± 0.03	-4.87
methyl_octanoate	-5.31 ± 0.01	2.37 ± 0.03	-2.94 ± 0.03	-2.04
methyl_p_methoxybenzoate	-7.45 ± 0.01	1.13 ± 0.03	-6.32 ± 0.03	-5.33
methyl_p_nitrobenzoate	-6.27 ± 0.01	-0.12 ± 0.03	-6.39 ± 0.03	-6.88
methyl_pentanoate	-5.43 ± 0.01	1.92 ± 0.02	-3.51 ± 0.02	-2.56
methyl_propanoate	-5.47 ± 0.01	1.64 ± 0.02	-3.83 ± 0.02	-2.93
methyl_propyl_ether	-2.76 ± 0.01	2.35 ± 0.02	-0.41 ± 0.02	-1.66
methyl_t_butyl_ether	-2.95 ± 0.01	2.35 ± 0.02	-0.60 ± 0.02	-2.21
methyl_tert_butyl_ether	-2.90 ± 0.01	2.22 ± 0.02	-0.68 ± 0.02	-2.21
methyl_trifluoroacetate	-3.40 ± 0.01	2.01 ± 0.02	-1.39 ± 0.02	-1.10
methyl_trimethylacetate	-5.28 ± 0.01	2.29 ± 0.02	-2.99 ± 0.02	-2.40
methylamine	-5.13 ± 0.01	1.69 ± 0.01	-3.44 ± 0.01	-4.55
methylcyclohexane	0.01 ± 0.00	1.81 ± 0.02	1.82 ± 0.02	1.70
methylcyclopentane	0.00 ± 0.00	2.12 ± 0.02	2.12 ± 0.02	1.59
morpholine	-6.62 ± 0.01	0.34 ± 0.02	-6.28 ± 0.02	-7.17
n_butane	0.01 ± 0.00	2.53 ± 0.02	2.54 ± 0.02	2.07
n_butanethiol	-2.39 ± 0.01	2.27 ± 0.02	-0.12 ± 0.02	-0.99
n_butyl_acetate	-5.45 ± 0.01	2.28 ± 0.02	-3.17 ± 0.02	-2.64
n_butylacetamide	-9.76 ± 0.02	1.62 ± 0.02	-8.14 ± 0.03	-9.31
n_butylamine	-5.11 ± 0.01	2.29 ± 0.02	-2.82 ± 0.02	-4.24
n_butylbenzene	-2.76 ± 0.01	2.46 ± 0.02	-0.30 ± 0.02	-0.40
n_decane	0.01 ± 0.00	3.42 ± 0.03	3.43 ± 0.03	3.16
n_heptane	0.01 ± 0.00	3.19 ± 0.02	3.20 ± 0.02	2.67
n_heptylamine	-4.89 ± 0.01	2.17 ± 0.03	-2.72 ± 0.03	-3.79
n_hexane	0.01 ± 0.00	3.04 ± 0.02	3.05 ± 0.02	2.48
n_hexyl_acetate	-5.49 ± 0.01	2.52 ± 0.03	-2.97 ± 0.03	-2.26
n_hexylamine	-4.88 ± 0.01	2.34 ± 0.02	-2.54 ± 0.02	-3.95
n_hexylbenzene	-2.71 ± 0.01	2.95 ± 0.03	0.24 ± 0.03	-0.04
n_nonane	0.01 ± 0.00	3.31 ± 0.03	3.32 ± 0.03	3.13

n_octane	0.01 ± 0.00	3.12 ± 0.03	3.13 ± 0.03	2.88
n_octylamine	-5.12 ± 0.01	2.74 ± 0.03	-2.38 ± 0.03	-3.65
n_pentane	0.01 ± 0.00	2.66 ± 0.02	2.67 ± 0.02	2.32
n_pentyl_acetate	-5.40 ± 0.01	2.57 ± 0.03	-2.83 ± 0.03	-2.51
n_pentyl_propanoate	-5.96 ± 0.01	2.60 ± 0.03	-3.36 ± 0.03	-2.11
n_pentylamine	-5.12 ± 0.01	2.13 ± 0.02	-2.99 ± 0.02	-4.09
n_pentylbenzene	-2.75 ± 0.01	2.80 ± 0.03	0.05 ± 0.03	-0.23
n_pentylcyclopentane	0.00 ± 0.00	2.39 ± 0.03	2.39 ± 0.03	2.55
n_propanethiol	-2.41 ± 0.01	2.10 ± 0.02	-0.31 ± 0.02	-1.06
n_propyl_acetate	-5.30 ± 0.01	1.97 ± 0.02	-3.33 ± 0.02	-2.79
n_propyl_butyrate	-5.35 ± 0.01	2.47 ± 0.03	-2.88 ± 0.03	-2.28
n_propyl_formate	-5.03 ± 0.01	1.53 ± 0.02	-3.50 ± 0.02	-2.48
n_propyl_propanoate	-5.45 ± 0.01	2.50 ± 0.02	-2.95 ± 0.02	-2.44
n_propylamine	-4.83 ± 0.01	1.78 ± 0.02	-3.05 ± 0.02	-4.39
n_propylbenzene	-2.72 ± 0.01	2.73 ± 0.02	0.01 ± 0.02	-0.53
n_propylcyclopentane	0.00 ± 0.00	2.15 ± 0.02	2.15 ± 0.02	2.13
naphthalene	-4.51 ± 0.01	1.17 ± 0.02	-3.34 ± 0.02	-2.40
nitrobenzene	-3.63 ± 0.01	0.23 ± 0.02	-3.40 ± 0.02	-4.12
nitroethane	-2.47 ± 0.01	0.74 ± 0.02	-1.73 ± 0.02	-3.71
nitromethane	-2.53 ± 0.01	0.50 ± 0.01	-2.03 ± 0.01	-4.02
non_1_ene	-0.33 ± 0.00	3.24 ± 0.03	2.91 ± 0.03	2.06
nonan_1_ol	-5.10 ± 0.01	2.56 ± 0.03	-2.54 ± 0.03	-3.88
nonan_2_one	-5.29 ± 0.01	2.78 ± 0.03	-2.51 ± 0.03	-2.49
nonan_5_one	-5.20 ± 0.01	2.86 ± 0.03	-2.34 ± 0.03	-2.64
nonanal	-5.09 ± 0.01	2.58 ± 0.03	-2.51 ± 0.03	-2.07
o_cresol	-6.55 ± 0.01	1.46 ± 0.02	-5.09 ± 0.02	-5.87
o_toluidine	-6.81 ± 0.02	1.44 ± 0.02	-5.37 ± 0.03	-5.53
o_xylene	-2.75 ± 0.01	2.23 ± 0.02	-0.52 ± 0.02	-0.90
oct_1_ene	-0.33 ± 0.00	3.10 ± 0.03	2.77 ± 0.03	1.92
oct_1_yne	-0.83 ± 0.00	3.29 ± 0.02	2.46 ± 0.02	0.71
octan_1_ol	-5.13 ± 0.01	2.48 ± 0.03	-2.65 ± 0.03	-4.09
octan_2_one	-5.31 ± 0.01	3.01 ± 0.03	-2.30 ± 0.03	-2.88
octanal	-5.12 ± 0.01	2.55 ± 0.03	-2.57 ± 0.03	-2.29
p_cresol	-6.95 ± 0.01	1.59 ± 0.02	-5.36 ± 0.02	-6.13
p_dibromobenzene	-1.70 ± 0.01	1.69 ± 0.02	-0.01 ± 0.02	-2.30
p_toluidine	-6.91 ± 0.02	1.35 ± 0.02	-5.56 ± 0.03	-5.57
p_xylene	-2.71 ± 0.01	2.04 ± 0.02	-0.67 ± 0.02	-0.80
pent_1_ene	-0.34 ± 0.00	2.78 ± 0.02	2.44 ± 0.02	1.68
pent_1_yne	-0.81 ± 0.01	2.74 ± 0.02	1.93 ± 0.02	0.01
penta_14_diene	-0.70 ± 0.00	2.88 ± 0.02	2.18 ± 0.02	0.93
pentachloroethane	-1.13 ± 0.01	1.44 ± 0.02	0.31 ± 0.02	-1.39
pentan_1_ol	-5.13 ± 0.01	1.99 ± 0.02	-3.14 ± 0.02	-4.57
pentan_2_ol	-5.19 ± 0.01	2.32 ± 0.02	-2.87 ± 0.02	-4.39
pentan_2_one	-5.25 ± 0.01	1.96 ± 0.02	-3.29 ± 0.02	-3.52
pentan_3_ol	-4.89 ± 0.01	1.94 ± 0.02	-2.95 ± 0.02	-4.35
pentan_3_one	-5.23 ± 0.01	2.29 ± 0.02	-2.94 ± 0.02	-3.41
pentanal	-5.08 ± 0.01	2.12 ± 0.02	-2.96 ± 0.02	-3.03
pentanenitrile	-3.56 ± 0.01	2.32 ± 0.02	-1.24 ± 0.02	-3.52
pentanoic_acid	-7.01 ± 0.06	1.64 ± 0.02	-5.37 ± 0.06	-6.16
phenanthrene	-6.00 ± 0.01	0.85 ± 0.03	-5.15 ± 0.03	-3.88
phenol	-7.01 ± 0.02	1.34 ± 0.02	-5.67 ± 0.03	-6.61
phenyl_formate	-6.26 ± 0.01	1.43 ± 0.02	-4.83 ± 0.02	-3.82
phenyl_methyl_sulfide	-3.14 ± 0.01	1.93 ± 0.02	-1.21 ± 0.02	-2.73
phenyl_trifluoroethyl_ether	-5.49 ± 0.01	2.56 ± 0.02	-2.93 ± 0.02	-1.29
piperazine	-8.72 ± 0.02	0.38 ± 0.02	-8.34 ± 0.03	-7.40
piperidine	-4.68 ± 0.01	1.22 ± 0.02	-3.46 ± 0.02	-5.11
prop_2_en_1_ol	-5.18 ± 0.02	1.95 ± 0.02	-3.23 ± 0.03	-5.03
propan_1_ol	-5.10 ± 0.01	1.98 ± 0.02	-3.12 ± 0.02	-4.85
propan_2_ol	-5.29 ± 0.01	2.01 ± 0.02	-3.28 ± 0.02	-4.74
propane	0.00 ± 0.00	2.56 ± 0.02	2.56 ± 0.02	1.96
propanenitrile	-3.61 ± 0.01	2.34 ± 0.02	-1.27 ± 0.02	-3.84

propanoic_acid	-7.64 ± 0.02	1.23 ± 0.02	-6.41 ± 0.03	-6.46
propanone	-5.31 ± 0.01	1.95 ± 0.02	-3.36 ± 0.02	-3.80
propene	-0.37 ± 0.00	2.81 ± 0.02	2.44 ± 0.02	1.32
propionaldehyde	-5.06 ± 0.01	1.98 ± 0.02	-3.08 ± 0.02	-3.43
propyne	-0.87 ± 0.00	2.66 ± 0.02	1.79 ± 0.02	-0.48
pyrene	-7.03 ± 0.01	0.41 ± 0.03	-6.62 ± 0.03	-4.52
pyridine	-4.75 ± 0.01	1.30 ± 0.02	-3.45 ± 0.02	-4.69
pyrrole	-5.16 ± 0.01	1.29 ± 0.02	-3.87 ± 0.02	-4.78
pyrrolidine	-4.89 ± 0.01	0.98 ± 0.02	-3.91 ± 0.02	-5.48
quinoline	-5.70 ± 0.01	0.83 ± 0.02	-4.87 ± 0.02	-5.72
sec_butylbenzene	-2.72 ± 0.01	2.76 ± 0.03	0.04 ± 0.03	-0.45
styrene	-3.34 ± 0.01	2.02 ± 0.02	-1.32 ± 0.02	-1.24
teflurane	-1.99 ± 0.01	2.45 ± 0.02	0.46 ± 0.02	0.50
tert_butylbenzene	-2.98 ± 0.01	2.56 ± 0.03	-0.42 ± 0.03	-0.44
tetrachloroethene	-0.09 ± 0.00	1.50 ± 0.02	1.41 ± 0.02	0.10
tetrachloromethane	-0.13 ± 0.00	1.54 ± 0.02	1.41 ± 0.02	0.08
tetrafluoromethane	-0.38 ± 0.00	2.80 ± 0.01	2.42 ± 0.01	3.12
tetrahydrofuran	-3.30 ± 0.01	1.23 ± 0.02	-2.07 ± 0.02	-3.47
tetrahydropyran	-2.80 ± 0.01	1.02 ± 0.02	-1.78 ± 0.02	-3.12
thiophene	-1.88 ± 0.01	1.54 ± 0.02	-0.34 ± 0.02	-1.42
thiophenol	-3.26 ± 0.01	1.83 ± 0.02	-1.43 ± 0.02	-2.55
toluene	-2.70 ± 0.01	1.99 ± 0.02	-0.71 ± 0.02	-0.89
trans_14_dimethylcyclohexane	0.01 ± 0.00	2.04 ± 0.02	2.05 ± 0.02	2.11
triacetyl_glycerol	-13.83 ± 0.08	0.52 ± 0.03	-13.31 ± 0.08	-8.84
tribromomethane	-0.70 ± 0.00	1.58 ± 0.02	0.88 ± 0.02	-2.13
trichloroethene	-0.82 ± 0.00	1.81 ± 0.02	0.99 ± 0.02	-0.44
trichloromethane	-1.23 ± 0.00	1.55 ± 0.02	0.32 ± 0.02	-1.08
triethyl_phosphate	-11.94 ± 0.02	1.88 ± 0.03	-10.06 ± 0.04	-7.54
triethylamine	-4.28 ± 0.01	2.45 ± 0.03	-1.83 ± 0.03	-3.22
trimethoxy_methane	-5.97 ± 0.02	1.91 ± 0.02	-4.06 ± 0.03	-4.42
trimethoxymethylbenzene	-7.42 ± 0.02	1.59 ± 0.03	-5.83 ± 0.04	-4.04
trimethyl_phosphate	-11.33 ± 0.02	0.74 ± 0.02	-10.59 ± 0.03	-8.70
trimethylamine	-4.15 ± 0.01	1.83 ± 0.02	-2.32 ± 0.02	-3.20
undecan_2_one	-5.26 ± 0.01	3.14 ± 0.03	-2.12 ± 0.03	-2.15

Table 2 shows the same quantities as in Table 1, but only for those compounds affected by the amended Lennard-Jones well depth for triple bonded carbons. The revised results are shown.

TABLE 2:: Computed and experimental hydration free energies and components.

Molecule name	$\Delta G_{elec.}$	$\Delta G_{vdw.}$	$\Delta G_{hyd.}$	$\Delta G_{expt.}$
333_trimethoxypropionitrile	-6.93 ± 0.02	1.19 ± 0.03	-5.74 ± 0.04	-6.40
3_cyanophenol	-8.08 ± 0.02	1.09 ± 0.02	-6.99 ± 0.03	-9.65
3_cyanopyridine	-5.84 ± 0.01	1.21 ± 0.02	-4.63 ± 0.02	-6.75
4_cyanophenol	-8.65 ± 0.02	1.41 ± 0.02	-7.24 ± 0.03	-10.17
4_cyanopyridine	-6.01 ± 0.01	1.00 ± 0.02	-5.01 ± 0.02	-6.02
acetonitrile	-3.76 ± 0.01	1.25 ± 0.01	-2.51 ± 0.01	-3.88
benzonitrile	-4.14 ± 0.01	1.52 ± 0.02	-2.62 ± 0.02	-4.21
but_1_yne	-0.77 ± 0.01	1.28 ± 0.02	0.51 ± 0.02	-0.16
butanenitrile	-3.59 ± 0.01	1.36 ± 0.02	-2.23 ± 0.02	-3.64
cyanobenzene	-4.13 ± 0.01	1.57 ± 0.02	-2.56 ± 0.02	-4.10
hept_1_yne	-0.75 ± 0.00	1.59 ± 0.02	0.84 ± 0.02	0.60
hex_1_yne	-0.76 ± 0.00	1.55 ± 0.02	0.79 ± 0.02	0.29
methyl_cyanoacetate	-6.86 ± 0.01	0.52 ± 0.02	-6.34 ± 0.02	-6.72
oct_1_yne	-0.75 ± 0.00	1.87 ± 0.03	1.12 ± 0.03	0.71
pent_1_yne	-0.74 ± 0.00	1.19 ± 0.02	0.45 ± 0.02	0.01
pentanenitrile	-3.58 ± 0.01	1.42 ± 0.02	-2.16 ± 0.02	-3.52
propyne	-0.79 ± 0.00	0.99 ± 0.01	0.20 ± 0.01	-0.48

Table 3 shows the conversion between the names as tabulated in this work and IUPAC names (generated from the mol2 files using OpenEye's Lexichem package).