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	$\Delta G_{elec.}$	ΔG_{vdw} .	ΔG_{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	$\frac{2.11 \pm 0.02}{2.27 \pm 0.02}$	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	2.13 ± 0.02 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	$\frac{1.61 \pm 0.02}{1.61 \pm 0.03}$	-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 2_chlorobutane	-6.04 ± 0.02	$\frac{1.08 \pm 0.02}{2.56 \pm 0.02}$	-4.96 ± 0.03	-4.91
	-1.35 ± 0.00	2.56 ± 0.02	1.21 ± 0.02	0.00
2_chlorophenol 2_chloropropane	$-4.51 \pm 0.02 -1.40 \pm 0.01$	1.28 ± 0.02 2.22 ± 0.02	-3.23 ± 0.03 0.82 ± 0.02	-4.55 -0.25
2_chloropyridine	-1.40 ± 0.01 -4.85 ± 0.01	2.22 ± 0.02 1.49 ± 0.02	-3.36 ± 0.02	-4.39
2_chlorotoluene	-4.85 ± 0.01 -2.18 ± 0.01	1.49 ± 0.02 1.67 ± 0.02	-3.36 ± 0.02 -0.51 ± 0.02	-1.14
2_ethoxyethanol	-2.18 ± 0.01 -6.41 ± 0.02	1.64 ± 0.02	-0.31 ± 0.02 -4.77 ± 0.03	-6.69
2_ethylpyrazine	-6.41 ± 0.02 -6.94 ± 0.02	1.04 ± 0.02 1.26 ± 0.02	-4.77 ± 0.03 -5.68 ± 0.03	-5.45
2_curyipyrazine	-0.94 ± 0.02	1.40 ± 0.02	-0.00 ± 0.03	-3.43

Zethytoluene	2_ethylpyridine	-4.96 ± 0.01	1.75 ± 0.02	-3.21 ± 0.02	-4.33
2.flotorophenol					
2.iodoppenol					
2.isobutylpyrazine					
2.isoluty pyrazine					
2.methoxy_111 trimethoxyethane					
2.methoxyenthanamine					
2.methoxyethanamine					
2.methylpentan -6.92 ± 0.02					
2.methylput.2.ene					
2.methylbut_2.ene					
2.methylbuta.1.3.diene					
2.methylputan.1.3.diene					
2.methylbutan.l.ol					
2.methylbutan.2.ol		-1.12 ± 0.01			
2.methylptentane					
2.methylpent.1 ene 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.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 2.450 2.methylpropan.2.ol -5.31 ± 0.01 2.22 ± 0.02 -3.09 ± 0.02 4.47 2.methylpropene -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 2.34 ± 0.02 2.methylpropene -0.45 ± 0.00 2.79 ± 0.02 2.34 ± 0.02 2.34 ± 0.02 2.methylpropene -0.49 ± 0.02 0.89 ± 0.02 -6.10 ± 0.03 -5.51 2.methylpropene -4.95 ± 0.01 1.54 ± 0.02 -3.41 ± 0.02 -4.33 2.methylprofure -1.90 ± 0.01 1.68 ± 0.02 -0.22 ± 0.02 -3.88 2.methylprofure -1.90					
2.methylpentan_2.ol					
2.methylpentan_2.ol -5.13 ± 0.01 2.34 ± 0.02 -2.79 ± 0.02 -3.92 2.methylpentan 0.01 ± 0.00 2.77 ± 0.02 2.56 ± 0.02 -2.19 ± 0.03 3.88 2.methylpropan_1.ol -5.02 ± 0.01 2.06 ± 0.02 2.78 ± 0.02 2.51 2.methylpropan_2.ol -5.31 ± 0.01 2.26 ± 0.02 -3.09 ± 0.02 -4.50 2.methylpropan 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.methylpropene -0.45 ± 0.00 2.73 ± 0.02 2.34 ± 0.02 1.16 2.methylpropene -0.45 ± 0.00 2.79 ± 0.02 2.34 ± 0.02 1.16 2.methylpridine -4.95 ± 0.01 1.54 ± 0.02 -3.41 ± 0.02 3.30 2.methylpropene -1.90 ± 0.01 1.64 ± 0.02 -1.95 ± 0.02 -3.30 2.methylpridine -1.90 ± 0.01 1.68 ± 0.02 -0.22 ± 0.02 -1.38 2.methylpridine -1.90 ± 0.01 1.68 ± 0.02 -7.88 ± 0.03 -7.87 2.methylpridine <					
2.methylpentan.3.ol -4.75 ± 0.02 2.56 ± 0.02 -2.19 ± 0.03 -3.88 2.methylpropan.1.ol -5.02 ± 0.01 2.06 ± 0.02 -2.78 ± 0.02 2.78 ± 0.02 2.51 2.methylpropan.2.ol -5.31 ± 0.01 2.22 ± 0.02 -2.30 ± 0.02 4.47 2.methylpropane 0.01 ± 0.00 2.73 ± 0.02 2.74 ± 0.02 2.32 2.methylpyrazine -6.99 ± 0.02 0.89 ± 0.02 -6.10 ± 0.03 -5.51 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.methylterahydrofuran -3.39 ± 0.01 1.68 ± 0.02 -0.22 ± 0.02 -3.30 2.methylterahydrofuran -8.70 ± 0.02 0.82 ± 0.02 -7.88 ± 0.03 -8.11 2.methylterahydrofuran -8.70 ± 0.02 0.82 ± 0.02 -7.88 ± 0.03 -8.11 2.nethylterahydrofuran -1.90 ± 0.01 1.68 ± 0.02 -7.28 ± 0.02 -1.88 ± 0.03 2.nethylterahydrofuran -8.70 ± 0.02 0.82 ± 0.02 -7.88 ± 0.03 -8.11 <					
2.methylpropan.1.ol 0.01 ± 0.00 2.77 ± 0.02 2.78 ± 0.02 2.51 2.methylpropan.2.ol -5.02 ± 0.01 2.06 ± 0.02 -2.96 ± 0.02 -4.50 2.methylpropane 0.01 ± 0.00 2.73 ± 0.02 2.74 ± 0.02 2.32 2.methylpropane -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 -4.60 2.methylthriophene -1.90 ± 0.01 1.68 ± 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.nitrophenol -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 -8.11 2.propoxyethanol -7.55 ± 0.02					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-4.75 ± 0.02			-3.88
$ \begin{array}{c} 2. \text{methylpropan.} 2. \text{ol} & -5.31 \pm 0.01 & 2.22 \pm 0.02 & -3.09 \pm 0.02 & -4.47 \\ 2. \text{methylpropane} & 0.01 \pm 0.00 & 2.73 \pm 0.02 & 2.74 \pm 0.02 & 2.32 \\ 2. \text{methylpropane} & -0.45 \pm 0.00 & 2.79 \pm 0.02 & 2.34 \pm 0.02 & 1.16 \\ 2. \text{methylpyrazine} & -6.99 \pm 0.02 & 0.89 \pm 0.02 & -6.10 \pm 0.03 & 5.51 \\ 2. \text{methylpyrazine} & -4.95 \pm 0.01 & 1.54 \pm 0.02 & -3.41 \pm 0.02 & -4.63 \\ 2. \text{methylterinydrofura} & -3.39 \pm 0.01 & 1.44 \pm 0.02 & -1.95 \pm 0.02 & -3.30 \\ 2. \text{methyltiophene} & -1.99 \pm 0.01 & 1.68 \pm 0.02 & -0.22 \pm 0.02 & -1.38 \\ 2. \text{naphthol} & -8.70 \pm 0.02 & 0.82 \pm 0.02 & -7.88 \pm 0.03 & -8.11 \\ 2. \text{naphthylamine} & -8.83 \pm 0.02 & 0.96 \pm 0.02 & -7.87 \pm 0.03 & -7.47 \\ 2. \text{nitroaniline} & -7.84 \pm 0.02 & -0.12 \pm 0.02 & -7.96 \pm 0.03 & -7.47 \\ 2. \text{nitropriphenol} & -5.40 \pm 0.02 & 0.06 \pm 0.02 & -5.34 \pm 0.03 & -4.58 \\ 2. \text{nitropropane} & -2.54 \pm 0.01 & 0.93 \pm 0.02 & -1.61 \pm 0.02 & -3.13 \\ 2. \text{nitrotoluene} & -3.79 \pm 0.01 & 0.65 \pm 0.02 & -3.14 \pm 0.02 & -3.58 \\ 2. \text{prepoxyethanol} & -7.05 \pm 0.02 & 1.72 \pm 0.02 & -5.33 \pm 0.03 & -6.79 \\ 2. \text{propoxyethanol} & -6.44 \pm 0.02 & 1.93 \pm 0.02 & -4.21 \pm 0.03 & -6.40 \\ 33. \text{dimethylpentane} & 0.01 \pm 0.00 & 2.52 \pm 0.03 & -4.93 \pm 0.04 & -6.40 \\ 33. \text{dimethylperione} & -6.88 \pm 0.02 & 1.95 \pm 0.03 & -4.93 \pm 0.04 & -6.40 \\ 33. \text{dimethylpyridine} & -6.86 \pm 0.02 & 1.53 \pm 0.02 & -5.33 \pm 0.03 & -6.50 \\ 34. \text{dimethylpyridine} & -6.86 \pm 0.02 & 1.53 \pm 0.02 & -5.33 \pm 0.03 & -6.50 \\ 34. \text{dimethylpyridine} & -4.79 \pm 0.01 & 1.63 \pm 0.02 & -5.33 \pm 0.03 & -6.50 \\ 34. \text{dimethylpyridine} & -4.79 \pm 0.01 & 1.53 \pm 0.02 & -5.33 \pm 0.03 & -6.50 \\ 34. \text{dimethylpyridine} & -6.86 \pm 0.02 & 1.53 \pm 0.02 & -5.33 \pm 0.03 & -5.51 \\ 35. \text{dimethylpyridine} & -6.86 \pm 0.02 & 1.53 \pm 0.02 & -5.33 \pm 0.03 & -5.51 \\ 35. \text{dimethylpyridine} & -4.79 \pm 0.01 & 1.61 \pm 0.02 & -5.33 \pm 0.03 & -5.51 \\ 3. \text{chloroprop.1.ene} & -1.48 \pm 0.01 & 1.04 \pm 0.02 & -5.37 \pm 0.02 & -5.82 \\ 3. \text{chloropropol.ene} & -1.48 \pm 0.01 & 1.04 \pm 0.02 & -5.37 \pm 0.02 & -5.82 \\ 3. \text{chloropropol.ene} & -1.48 \pm 0.01 & 1.38 \pm 0.02 & -5.02 \pm 0.03 $	2_methylpentane	0.01 ± 0.00	2.77 ± 0.02	2.78 ± 0.02	2.51
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.methylthiophene -1.90 ± 0.01 1.68 ± 0.02 -0.22 ± 0.02 -1.38 2.maphthol -8.70 ± 0.02 0.82 ± 0.02 -7.88 ± 0.03 -8.11 2.naphthylamine -8.83 ± 0.02 0.96 ± 0.02 -7.88 ± 0.03 -7.47 2.nitroaniline -7.84 ± 0.02 -0.12 ± 0.02 -7.96 ± 0.03 -7.47 2.nitrophenol -5.40 ± 0.02 0.06 ± 0.02 -5.34 ± 0.03 -7.37 2.nitroptopane -2.54 ± 0.01 0.93 ± 0.02 -1.61 ± 0.02 -3.13 2.nitroptoune -3.79 ± 0.01 0.65 ± 0.02 -5.33 ± 0.03 -6.79 2.phenylethanol -7.05 ± 0.02 1.72 ± 0.02 -5.33 ± 0.03 -6.79 2.phenylethanol -6.14 ± 0.02 1.9	2_methylpropan_1_ol	-5.02 ± 0.01	2.06 ± 0.02	-2.96 ± 0.02	-4.50
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2_methylpropan_2_ol	-5.31 ± 0.01	2.22 ± 0.02	-3.09 ± 0.02	-4.47
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2_methylpropane	0.01 ± 0.00	2.73 ± 0.02	2.74 ± 0.02	2.32
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_nitrotoluene -3.79 ± 0.01 0.65 ± 0.02 -3.14 ± 0.02 -3.13 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 33_dimethylptana_2_one -5.18 ± 0.01 2.27 ± 0.02 -2.33 ± 0.03 -6.79 2_propoxyethanol -6.14 ± 0.02 1.93 ± 0.02 -4.21 ± 0.03 -6.40 3_dimethylptana -0.11 ± 0.	2_methylpropene	-0.45 ± 0.00	2.79 ± 0.02	2.34 ± 0.02	1.16
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2_methylpyrazine	-6.99 ± 0.02	0.89 ± 0.02	-6.10 ± 0.03	-5.51
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-4.95 ± 0.01	1.54 ± 0.02	-3.41 ± 0.02	-4.63
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					-1.38
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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_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_methyl_but_1_ene -0.33 ± 0.00 3.13 ± 0.02 2.80 ± 0.02 1.83					
3_methylbut_1_ene $ -0.34 \pm 0.00 3.01 \pm 0.02 2.67 \pm 0.02 1.82 $					
	3_methylbut_1_ene	-0.34 ± 0.00	3.01 ± 0.02	2.67 ± 0.02	1.82

3.methylbutun.2.one	3_methylbutan_1_ol	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-4.42
3.methylbatanoic acid					
3.methylheptane					
3.methylpexame					
3.methylpentane					
3.methylpyridine					
3.nitrophenol					
3.nitrophenol					
3.nitrotoluene					
3.phenylpropanol					
4.aetylpyridine					
4.bromothelune					
A. Demontoluene					
4.chloro.3.methylphenol -6.38 ± 0.02 1.48 ± 0.02 -4.90 ± 0.03 -6.79 4.chlorophenol -6.47 ± 0.01 1.19 ± 0.02 -5.28 ± 0.02 -5.99 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.ethylpydidine -4.72 ± 0.01 1.85 ± 0.02 -2.87 ± 0.02 -4.73 4.ethylpyridine -6.51 ± 0.02 1.55 ± 0.02 -4.99 ± 0.03 -6.19 4.fluorophenol -6.51 ± 0.02 1.52 ± 0.02 -4.99 ± 0.03 -6.19 4.fluorophenol -6.51 ± 0.02 1.52 ± 0.02 -4.99 ± 0.03 -6.19 4.fluorophenol -6.51 ± 0.02 0.82 ± 0.02 -7.31 ± 0.03 -7.09 4.fluorophenol -7.89 ± 0.01 1.60 ± 0.03 -6.29 ± 0.03 -4.09 4.speroxylitoluen -7.89 ± 0.01 1.60 ± 0.03 -6.29 ± 0.03 -4.78 4.methylacylitolue -8.50 ± 0.02 <td></td> <td></td> <td></td> <td></td> <td></td>					
4.chlorophenol -6.47 ± 0.01 1.19 ± 0.02 -5.28 ± 0.02 -5.90 4.cyanophenol -8.73 ± 0.02 1.11 ± 0.02 -5.36 ± 0.02 -7.03 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.ethylpridine -4.72 ± 0.01 1.85 ± 0.02 -2.87 ± 0.02 -4.93 4.ethylpridine -2.78 ± 0.01 2.73 ± 0.02 -0.05 ± 0.02 -4.93 4.flormylpridine -8.13 ± 0.02 0.82 ± 0.02 -7.31 ± 0.03 -6.19 4.formylpridine -8.13 ± 0.02 0.85 ± 0.02 -7.31 ± 0.03 -7.00 4.sporpyltoluene -2.53 ± 0.01 2.73 ± 0.03 0.20 ± 0.03 8.83 4.isporpyltoluene -7.89 ± 0.01 1.66 ± 0.03 -6.29 ± 0.03 4.40 4.methoxyactophenone -7.89 ± 0.01 1.66 ± 0.03 -6.29 ± 0.03 4.74 4.methylenia -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 1.02 4.methylentan 2.oi -6.70 ± 0.02					
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 -0.17 4.cyanophenol -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 -9.95 4.flormylpyridine -8.13 ± 0.02 1.52 ± 0.02 -4.99 ± 0.03 -6.19 4.flormylpyridine -8.13 ± 0.02 0.82 ± 0.02 -7.31 ± 0.03 -7.00 4.flormylpyridine -10.85 ± 0.02 0.85 ± 0.02 -7.31 ± 0.03 -7.00 4.mydroxybenzaldehyde -10.85 ± 0.02 0.85 ± 0.02 -7.31 ± 0.03 -7.00 4.methylpentone -2.53 ± 0.01 2.73 ± 0.03 0.20 ± 0.03 -6.88 4.methyll.h.imidazole -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 -10.27 4.methylpentan 2.ol -5.10 ± 0.01 2.35 ± 0.02 -7.55 ± 0.02 3.37 4.methylpentan 2.ol -5.					
4.cyanopyridine					
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.ethylphenol -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.flourophenol -6.61 ± 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 -7.48 4.methyl.l.inidazole -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 -10.27 4.methylpentan 2.ol -6.71 ± 0.02 1.88 ± 0.02 -4.82 ± 0.03 -4.72 4.methylpentaln 2.ol -5.28 ± 0.01 2.35 ± 0.02 -2.96 ± 0.02 -3.73 4.methylpentaln 2.ol					
4.ethylphenol -7.07 ± 0.02 1.99 ± 0.02 -5.08 ± 0.03 -6.13 4.ethylpytidine -4.72 ± 0.01 1.85 ± 0.02 -2.87 ± 0.02 -9.50 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -0.95 -0.02 -1.03 -7.00 -0.03 -6.19 4.00 -1.08 -1.08 -1.08 -1.08 -1.08 -1.08 -1.00 -0.03 -8.03 -8.03 -1.00 -0.03 -8.03 -8.08 4.00 -8.55 0.02 -1.17 0.03 -6.29 0.03 -4.06 4.08 4.08 4.00 -1.17 0.03 -6.29 0.03 -4.04 4.06 4.06 4.03 -6.92 0.03 -7.29 0.03 -4.02 4.06 4.02 4.02 4.82 0.03 -4.02 4.02					
4.ethylpyridine -4.72 ± 0.01 1.85 ± 0.02 -2.87 ± 0.02 -0.05 -0.95 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 1.60 ± 0.03 -6.29 ± 0.03 -4.06 4.methoxyacetophenone -7.89 ± 0.01 1.60 ± 0.03 -6.29 ± 0.03 -7.48 4.methyl.1h.imidazole -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 -7.48 4.methylacetophenone -6.70 ± 0.02 1.88 ± 0.02 -4.89 ± 0.03 -4.73 4.methylpentan-2.ol -5.10 ± 0.01 2.35 ± 0.02 -2.75 ± 0.03 -7.78 4.methylpentan-2.one -5.28 ± 0.01 2.32 ± 0.02 -2.75 ± 0.02 -3.03 4.methylpentan-2.one -6.96 ± 0.01 1.36 ± 0.02 -2.3 ± 0.02 -2.5 ± 0.02 -3.04					
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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 1.60 ± 0.03 -0.29 ± 0.03 -4.40 4.methoxyactophenone -7.89 ± 0.01 1.60 ± 0.03 -6.29 ± 0.03 -4.40 4.methyl.1h.imidazole -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 -7.48 4.methylacetophenone -6.70 ± 0.02 1.88 ± 0.02 -4.82 ± 0.03 -4.70 4.methylpentan2.ol -6.43 ± 0.02 1.53 ± 0.02 -4.90 ± 0.03 -4.27 4.methylppridine -4.73 ± 0.01 2.35 ± 0.02 -2.75 ± 0.02 -3.05 4.methylpyridine -4.73 ± 0.01 1.32 ± 0.02 -2.96 ± 0.02 -3.05 4.nitrophenol -6.96 ± 0.01 1.46 ± 0.02 -5.50 ± 0.02 -5.90 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.but_2.enal					
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 -6.29 ± 0.03 -7.48 4.methyl.1h.imidazole -8.85 ± 0.02 0.86 ± 0.02 -7.99 ± 0.03 -10.27 4.methylbenzaldehyde -6.70 ± 0.02 1.88 ± 0.02 -4.82 ± 0.03 -4.70 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.methylppridine -4.73 ± 0.01 1.32 ± 0.02 -3.41 ± 0.02 -4.32 4.n.propylphenol -6.66 ± 0.01 1.46 ± 0.02 -5.50 ± 0.02 -5.90 4.nitrophenol -8.04 ± 0.01 -0.18 ± 0.02 -8.23 ± 0.02 -10.64 4.tert.butylphenol -7.21 ± 0.02 1.67 ± 0.03 -5.54 ± 0.04 -5.91 4.pet.2.enal			0.82 ± 0.02		
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			2.73 ± 0.03		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				-6.29 ± 0.03	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		-8.09 ± 0.02	1.17 ± 0.02	-6.92 ± 0.03	-7.48
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			0.86 ± 0.02	-7.99 ± 0.03	-10.27
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					-4.70
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_methylbenzaldehyde	-6.43 ± 0.02	1.53 ± 0.02	-4.90 ± 0.03	-4.27
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_methylpentan_2_ol	-5.10 ± 0.01	2.35 ± 0.02	-2.75 ± 0.02	-3.73
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_methylpentan_2_one	-5.28 ± 0.01	2.32 ± 0.02	-2.96 ± 0.02	-3.05
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_methylpyridine	-4.73 ± 0.01	1.32 ± 0.02	-3.41 ± 0.02	-4.93
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_n_propylphenol	-6.96 ± 0.01	1.46 ± 0.02	-5.50 ± 0.02	-5.90
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_nitroaniline	-9.03 ± 0.02	-0.20 ± 0.02	-9.23 ± 0.03	-10.27
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4_nitrophenol	-8.04 ± 0.01	-0.18 ± 0.02	-8.22 ± 0.02	-10.64
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		-7.21 ± 0.02	1.67 ± 0.03	-5.54 ± 0.04	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	E_12_dichloroethene	-0.87 ± 0.00	2.07 ± 0.02	1.20 ± 0.02	-0.78
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	E_but_2_enal	-5.82 ± 0.01	2.16 ± 0.02	-3.66 ± 0.02	-4.22
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	E_hept_2_ene	-0.43 ± 0.00	3.26 ± 0.02	2.83 ± 0.02	1.68
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	E_hex_2_enal	-5.48 ± 0.01	2.26 ± 0.02	-3.22 ± 0.02	-3.68
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			-0.68 ± 0.03		
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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					
acenaphthene $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					
acetaldehyde -5.18 ± 0.01 1.79 ± 0.02 -3.39 ± 0.02 -3.50					
acetic_acid $ -7.07 \pm 0.02 1.12 \pm 0.01 -5.95 \pm 0.02 -6.69 $					
·	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	-3.37 ± 0.01 -4.97 ± 0.01	1.51 ± 0.02 1.58 ± 0.02	-3.39 ± 0.02	-2.66
bis_2_chloroethylether	-3.78 ± 0.01	1.92 ± 0.02	-3.39 ± 0.02 -1.86 ± 0.02	-4.23
bromoethane	-2.20 ± 0.01	1.83 ± 0.02	-0.37 ± 0.02	-1.46
***************************************	-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	-5.28 ± 0.01 -5.14 ± 0.01	1.02 ± 0.02 1.30 ± 0.02	-4.20 ± 0.02 -3.84 ± 0.02	-4.91
cyclohexene	-0.53 ± 0.00	2.09 ± 0.02	$\frac{-3.64 \pm 0.02}{1.56 \pm 0.02}$	0.37
cyclohexylamine	-5.08 ± 0.00	1.14 ± 0.02	-3.94 ± 0.02	-4.59
cyclopentane	-3.03 ± 0.01 0.01 ± 0.00	1.14 ± 0.02 1.52 ± 0.02	$\frac{-3.94 \pm 0.02}{1.53 \pm 0.02}$	1.20
cyclopentanol	-5.27 ± 0.01	1.52 ± 0.02 1.12 ± 0.02	-4.15 ± 0.02	-5.49
cyclopentanoi				
	-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
	1			

dethoty, distribution -7.19 ± 0.02 2.7.5 ± 0.03 -4.44 ± 0.04 -2.9 1.64 diethyl, destribution -2.51 ± 0.01 2.32 ± 0.02 -0.71 ± 0.02 -1.54 diethyl, ether -3.02 ± 0.01 1.82 ± 0.03 -0.45 ± 0.04 5.71 diethyl, succinate -10.32 ± 0.02 1.85 ± 0.03 -8.47 ± 0.04 5.71 diethyl, succinate -10.32 ± 0.02 2.18 ± 0.01 2.39 ± 0.02 0.21 ± 0.02 -1.46 distyl, succinate -4.93 ± 0.01 1.56 ± 0.02 -0.71 ± 0.02 -1.46 distyl, succinate -4.93 ± 0.01 1.56 ± 0.02 -0.71 ± 0.02 -4.73 distyl, succinate -4.33 ± 0.01 1.56 ± 0.02 -0.71 ± 0.02 -2.49 discoppost, succinate -3.01 ± 0.01 2.50 ± 0.02 -1.19 ± 0.02 -2.33 diisoprospl. teher -3.01 ± 0.01 2.50 ± 0.02 -1.91 ± 0.02 -3.22 dimethyl, disulfide -0.72 ± 0.00 2.20 ± 0.02 1.48 ± 0.02 -1.83 dimethyl, sulfoste -1.72 ± 0.01 1.85 ± 0.02 -7.85 ± 0.02 -1.61 <th>12 41 41 1</th> <th>7.10 0.00</th> <th>0.75 0.00</th> <th>4.44 0.04</th> <th>5.00</th>	12 41 41 1	7.10 0.00	0.75 0.00	4.44 0.04	5.00
diethyl nehr -3.02±0.01 2.32±0.02 -0.70±0.02 -1.59 diethyl malonate -8.27±0.02 1.85±0.03 -6.45±0.04 -6.00 diethyl susified -2.18±0.01 2.39±0.02 0.21±0.02 -1.46 diethyl sulfide -2.18±0.01 2.39±0.02 -2.72±0.02 -1.46 diethylamine -4.03±0.01 1.56±0.02 -7.73±0.02 -2.49 diisopropyl. ether -3.01±0.01 2.90±0.02 -0.11±0.02 -5.33 diisopropylamine -4.60±0.01 2.63±0.02 -1.19±0.02 -5.33 diimethyl sulfide -0.72±0.00 2.20±0.02 -1.48±0.02 -3.83 diimethyl sulfide -1.70±0.01 1.85±0.02 -1.88±0.02 -1.91 dimethyl sulfide -1.70±0.01 1.96±0.02 -2.83±0.03 -8.71 dimethyl sulfide -1.70±0.01 1.96±0.02 -2.83±0.03 -8.71 dimethyl sulfore -1.21±0.02 0.85±0.02 -0.83±0.03 -8.71 dimethyl sulfore -1.21±0.02 0.85±0.02 -2.83±0.03 -8.7	diethoxymethoxybenzene	-7.19 ± 0.02	2.75 ± 0.03	-4.44 ± 0.04	-5.23
diethyl malonate -8.27 ± 0.02 1.82 ± 0.03 -6.15 ± 0.04 -5.07 diethyl sucinite -10.32 ± 0.02 1.85 ± 0.03 -8.47 ± 0.04 5.71 diethyl sudifide -2.18 ± 0.01 2.23 ± 0.02 -2.72 ± 0.02 -1.46 diethylamine -4.93 ± 0.01 2.21 ± 0.02 -2.72 ± 0.02 -4.07 diisopropyl ether -3.01 ± 0.01 2.90 ± 0.02 -0.11 ± 0.02 -0.53 diisopropyl ether -3.01 ± 0.01 2.63 ± 0.02 -1.97 ± 0.02 -3.2 diisopropyl ether -4.06 ± 0.01 2.63 ± 0.02 -1.11 ± 0.02 -0.53 diimethyl disulfide -0.72 ± 0.00 1.86 ± 0.02 -1.85 ± 0.02 -1.83 dimethyl sulfide -0.72 ± 0.00 1.85 ± 0.02 -1.85 ± 0.02 -1.81 dimethyl sulfode -1.12 ± 0.02 0.85 ± 0.02 -7.85 ± 0.02 -5.10 dimethyl sulfode -9.48 ± 0.02 1.36 ± 0.02 -8.25 ± 0.02 -5.10 dimethyl sulfode -9.48 ± 0.02 1.36 ± 0.02 -8.25 ± 0.03 8.81 dimethyl sulfoxide -9.48 ±					
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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 -1.08 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 -8.62 ± 0.03 -9.71 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 1.18 ethanol -5.20 ± 0.02 1.75 ± 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 2.24 ethyl buroate -6.33 ± 0.01 1.65 ± 0.02 -4.68 ± 0.02 2.64 ethyl buroate -5.39 ± 0.01 1.53 ± 0.02 -3.04 ± 0.02 2.24 ethyl buroate -5.43 ± 0.02 2.63 ± 0.03 -2.89 ± 0.02 2.56		-2.70 ± 0.01	1.85 ± 0.02		-1.91
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 dimethyl.sulfoxide -9.94 ± 0.02 1.32 ± 0.02 -8.62 ± 0.03 -8.71 ethane 0.00 ± 0.00 2.58 ± 0.01 2.58 ± 0.01 1.83 ethane 0.00 ± 0.01 2.99 ± 0.02 -4.04 ± 0.02 -1.14 ethanethiol -5.20 ± 0.02 1.75 ± 0.02 -3.45 ± 0.03 -5.00 ethanol -5.20 ± 0.02 1.75 ± 0.02 -3.45 ± 0.03 -5.00 ethyl.ectate -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 -2.99 0.02 -2.66 ethyl.benzoate -5.43 ± 0.02 2.63 ± 0.03 -2.80 ± 0.04 -2.23 ethyl.benzoat -5.47 ± 0.01 2.15 ± 0.02 -3.04 ± 0.02 -2.99 0.02 -2.66 ethyl.benzoat -5.		-8.13 ± 0.01	0.28 ± 0.02	-7.85 ± 0.02	
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 ethanel -0.00 ± 0.00 2.58 ± 0.01 2.58 ± 0.01 1.83 ethanel -0.00 ± 0.00 2.06 ± 0.01 2.35 ± 0.02 -0.40 ± 0.02 1.18 ethandol -5.20 ± 0.02 1.75 ± 0.02 -3.45 ± 0.03 5.50 ethen -0.30 ± 0.00 2.66 ± 0.01 2.36 ± 0.01 1.28 ethyl_actate -5.14 ± 0.01 1.91 ± 0.02 -3.23 ± 0.02 -2.94 ethyl_botanoate -5.39 ± 0.01 2.35 ± 0.02 -3.04 ± 0.02 -2.94 ethyl_benzoate -5.47 ± 0.01 2.38 ± 0.03 -3.09 ± 0.02 -2.56 ethyl_entanoate -5.47 ± 0.01 2.13 ± 0.02 -2.99 ± 0.02 -2.5 ethyl_entanoate -5.47 ± 0.01 2.11 ± 0.02		-1.70 ± 0.01	1.96 ± 0.02		-1.61
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.formate -4.52 ± 0.01 1.53 ± 0.02 -3.04 ± 0.02 -2.49 ethyl.formate -4.52 ± 0.01 1.53 ± 0.02 -3.09 ± 0.03 -2.49 ethyl.phanylether -4.12 ± 0.01 2.11 ± 0.02 -2.99 ± 0.02 -2.56 ethyl.phenylether -4.12 ± 0.01 2.11 ± 0.02 -2.01 ± 0.02 -2.22 ethyl.propanoate -5.51 ± 0.01 2.11 ± 0.02 -3.39 ± 0		-11.21 ± 0.02		-10.36 ± 0.03	
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 ethanehiol -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.benzoate -5.14 ± 0.01 1.91 ± 0.02 -3.23 ± 0.02 -2.94 ethyl.benzoate -6.33 ± 0.01 1.28 ± 0.02 -3.04 ± 0.02 -2.94 ethyl.butanoate -5.39 ± 0.01 2.35 ± 0.02 -3.04 ± 0.02 -2.94 ethyl.pentanoate -5.43 ± 0.02 2.63 ± 0.03 -3.99 ± 0.02 -2.56 ethyl.pentanoate -5.47 ± 0.01 2.13 ± 0.02 -2.99 ± 0.02 -2.56 ethyl.pentanoate -5.47 ± 0.01 2.12 ± 0.02 -3.39 ± 0.04 -2.23 ethyl.pentanoate -5.51 ± 0.01 2.11 ± 0.02 -2.01 ± 0.02 -2.59 ethyl.pentanoate -5.51 ± 0.01 2.12 ± 0.02 -3		-9.68 ± 0.02		-8.32 ± 0.03	-8.71
$\begin{array}{c} \text{ethane} \\ \text{ethanethiol} \\ \text{ethanethiol} \\ \text{chanotl} \\ \text{delanethiol} \\ \text{chanotl} \\ \text{delanethiol} \\ \text{chanotl} \\ \text{chyl.butanoate} \\ \text{chyl.butanoate} \\ \text{chyl.butanoate} \\ \text{chyl.bexanoate} \\ \text{chyl.bexanoate} \\ \text{chyl.phenyl.chter} \\ \text{chyl.phenyl.chter} \\ \text{chyl.phenyl.chter} \\ \text{chyl.phenyl.chter} \\ \text{chyl.propanoate} \\ \text{chyl.propanote} \\ \text{chyl.propanoate} \\ \text{chyl.propanoate} \\ \text{chyl.propanoate} \\ \text{chyl.propanote} \\ \text{chyl.propanoate} \\ \text{chyl.propanote} \\ chy$				-3.11 ± 0.02	-4.29
$\begin{array}{c} \text{ethanethiol} \\ \text{ethanol} \\ \text{chanol} \\ \text{cheme} \\ \text{cheme} \\ \text{chor} \\ \text{chor} \\ \text{cheme} \\ \text{chor} \\ ch$	ethanamide	-9.94 ± 0.02	1.32 ± 0.02	-8.62 ± 0.03	-9.71
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 cthyl_benzoate -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_bulanoate -5.39 ± 0.01 2.35 ± 0.02 -3.04 ± 0.02 -2.99 ethyl_formate -4.52 ± 0.01 1.53 ± 0.02 -2.99 ± 0.02 -2.56 ethyl_pentanoate -5.47 ± 0.01 2.38 ± 0.03 -2.80 ± 0.04 -2.23 ethyl_phenyl_ether -4.12 ± 0.01 2.11 ± 0.02 -2.01 ± 0.02 -2.29 ethyl_phenyl_ether -4.12 ± 0.01 2.21 ± 0.02 -3.39 ± 0.03 -2.49 ethyl_phenyl_ether -4.12 ± 0.01 2.21 ± 0.02 -3.39 ± 0.03 -2.49 ethyl_phenyl_ether -4.12 ± 0.01 2.11 ± 0.02 -3.01 ± 0.02 -2.29 ethyl_phenyl_ether -4.12 ± 0.01 2.12 ± 0.02 -3.39 ± 0.02 -2.69 ethyl_phenyl_ether -5.00 ± 0.01	ethane	0.00 ± 0.00	2.58 ± 0.01	2.58 ± 0.01	1.83
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	ethanethiol	-2.49 ± 0.01	2.09 ± 0.02	-0.40 ± 0.02	-1.14
$\begin{array}{c} \text{ethyl.acetate} & -5.14 \pm 0.01 & 1.91 \pm 0.02 & -3.23 \pm 0.02 & -2.94 \\ \text{ethyl.benzoate} & -6.33 \pm 0.01 & 1.65 \pm 0.02 & -4.68 \pm 0.02 & -3.64 \\ \text{ethyl.butanoate} & -5.39 \pm 0.01 & 1.53 \pm 0.02 & -3.04 \pm 0.02 & -2.49 \\ \text{ethyl.formate} & -4.52 \pm 0.01 & 1.53 \pm 0.02 & -2.99 \pm 0.02 & -2.56 \\ \text{ethyl.hexanoate} & -5.43 \pm 0.02 & 2.63 \pm 0.03 & -2.80 \pm 0.04 & -2.23 \\ \text{ethyl.pentanoate} & -5.47 \pm 0.01 & 2.33 \pm 0.03 & -3.09 \pm 0.03 & -2.49 \\ \text{ethyl.pentanoate} & -5.47 \pm 0.01 & 2.33 \pm 0.03 & -3.09 \pm 0.03 & -2.49 \\ \text{ethyl.phenyl.ether} & -4.12 \pm 0.01 & 2.11 \pm 0.02 & -2.01 \pm 0.02 & -2.22 \\ \text{ethyl.propanoate} & -5.51 \pm 0.01 & 2.11 \pm 0.02 & -2.01 \pm 0.02 & -2.68 \\ \text{ethyl.mine} & -5.00 \pm 0.01 & 1.86 \pm 0.02 & -3.14 \pm 0.02 & -4.50 \\ \text{ethylbenzene} & -2.76 \pm 0.01 & 2.17 \pm 0.02 & -0.59 \pm 0.02 & -0.79 \\ \text{fluorone} & -5.31 \pm 0.01 & 1.02 \pm 0.02 & -4.29 \pm 0.02 & -3.35 \\ \text{fluorobenzene} & -2.10 \pm 0.01 & 2.03 \pm 0.02 & -0.07 \pm 0.02 & -0.80 \\ \text{fluoromethane} & -1.61 \pm 0.01 & 2.40 \pm 0.01 & 0.79 \pm 0.01 & -0.22 \\ \text{formaldehyde} & -4.87 \pm 0.01 & 1.65 \pm 0.01 & -3.22 \pm 0.01 & -2.25 \\ \text{hept.l.ene} & -0.33 \pm 0.00 & 3.30 \pm 0.02 & 2.97 \pm 0.02 & -0.11 \\ \text{hept.l.yne} & -0.80 \pm 0.00 & 3.80 \pm 0.02 & 2.28 \pm 0.02 & 0.60 \\ \text{hept.l.yne} & -0.80 \pm 0.00 & 3.80 \pm 0.02 & 2.28 \pm 0.02 & -0.01 \\ \text{heptan.2.one} & -5.30 \pm 0.01 & 2.50 \pm 0.02 & -2.80 \pm 0.02 & -3.04 \\ \text{heptan.4.one} & -5.99 \pm 0.01 & 2.51 \pm 0.02 & -2.280 \pm 0.02 & -2.92 \\ \text{hexanla} & -5.06 \pm 0.01 & 2.43 \pm 0.03 & -2.63 \pm 0.03 & -2.67 \\ \text{hex.1.ene} & -0.33 \pm 0.00 & 2.91 \pm 0.02 & 2.29 \pm 0.02 & -3.04 \\ \text{hexanl.od} & -5.08 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.92 \\ \text{hexan.l.od} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.80 \pm 0.02 & -3.04 \\ \text{hexanl.od} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.92 \\ \text{hexan.l.od} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.92 \\ \text{hexan.l.od} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.92 \\ \text{hexan.l.od} & -5.08 \pm 0.01 & 2.05 \pm 0.02 & -3.03 \pm 0.02 & -4.40 \\ \text{hexan.l.od} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -3.04 \\ \text{hexan.l.od} & -5.9$	ethanol	-5.20 ± 0.02	1.75 ± 0.02	-3.45 ± 0.03	-5.00
$\begin{array}{c} \text{ethyl.benzoate} \\ \text{ethyl.butanoate} \\ \text{colspit.butanoate} \\ \text{colspit.butanoate}$	ethene	-0.30 ± 0.00	2.66 ± 0.01	2.36 ± 0.01	
$\begin{array}{c} \text{ethyl.benzoate} \\ \text{ethyl.butanoate} \\ \text{colspit.butanoate} \\ \text{colspit.butanoate}$	ethyl_acetate	-5.14 ± 0.01	1.91 ± 0.02	-3.23 ± 0.02	-2.94
$\begin{array}{c} \text{ethyl.butanoate} \\ \text{ethyl.formate} \\ \text{cthyl.hexanoate} \\ ct$			1.65 ± 0.02		
$\begin{array}{c} \text{ethyl.formate} \\ \text{ethyl.hexanoate} \\ \text{ethyl.hexanoate} \\ \text{ethyl.pentanoate} \\ \text{ethyl.pentanoate} \\ \text{ethyl.pentanoate} \\ \text{ethyl.pentyl.ether} \\ \text{ethyl.pentyl.ether} \\ \text{ethyl.phenyl.ether} \\ \text{ethyl.propanoate} \\ ethyl.propan$					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					
$ \begin{array}{c} \text{ethyl.pentanoate} \\ \text{ethyl.phenyl.ether} \\ \text{cthyl.phenyl.ether} \\ \text{cthyl.phenyl.ether} \\ \text{cthyl.propaneate} \\ cthyl.$					
$\begin{array}{c} \text{ethyl.phenyl.ether} \\ \text{ethyl.propanoate} \\ \text{cthylamine} \\ cthylam$					
$ \begin{array}{c} \text{ethyl.propanoate} \\ \text{ethylamine} \\ \text{o} -5.51 \pm 0.01 \\ \text{o} 1.86 \pm 0.02 \\ \text{o} -3.14 \pm 0.02 \\ \text{o} -3.14 \pm 0.02 \\ \text{o} -4.50 \\ \text{ethylbenzene} \\ \text{o} -2.76 \pm 0.01 \\ \text{o} 1.86 \pm 0.02 \\ \text{o} -3.14 \pm 0.02 \\ \text{o} -3.14 \pm 0.02 \\ \text{o} -4.50 \\ \text{o} \\ \text{o} -2.76 \pm 0.01 \\ \text{o} -2.76 \pm 0.01 \\ \text{o} -2.76 \pm 0.01 \\ \text{o} -2.02 \\ \text{o} -0.59 \pm 0.02 \\ \text{o} \\ \text{o} -3.55 \\ \text{fluorobenzene} \\ \text{o} -2.10 \pm 0.01 \\ \text{o} -2.03 \pm 0.02 \\ \text{o} -0.07 \pm 0.02 \\ \text{o} \\ \text{o} -3.85 \\ \text{fluoromethane} \\ \text{o} -1.61 \pm 0.01 \\ \text{o} -3.01 \\ \text{o} -3.02 \pm 0.01 \\ \text{o} \\ \text{o} -3.22 \pm 0.01 \\ \text{o} \\ \text{o} \\ \text{o} \\ \text{o} \\ \text{o} \\ \text{o} \\ \text{fluoromethane} \\ \text{o} -1.61 \pm 0.01 \\ \text{o} \\$					
$\begin{array}{c} \text{ethylamine} & -5.00 \pm 0.01 & 1.86 \pm 0.02 & -3.14 \pm 0.02 & -4.50 \\ \text{ethylbenzene} & -2.76 \pm 0.01 & 2.17 \pm 0.02 & -0.59 \pm 0.02 & -0.79 \\ \text{fluorene} & -5.31 \pm 0.01 & 1.02 \pm 0.02 & -4.29 \pm 0.02 & -3.35 \\ \text{fluorobenzene} & -2.10 \pm 0.01 & 2.03 \pm 0.02 & -0.07 \pm 0.02 & -0.80 \\ \text{fluoromethane} & -1.61 \pm 0.01 & 2.40 \pm 0.01 & 0.79 \pm 0.01 & -0.22 \\ \text{formaldehyde} & -4.87 \pm 0.01 & 1.65 \pm 0.01 & -3.22 \pm 0.01 & -2.75 \\ \text{halothane} & -1.59 \pm 0.01 & 2.29 \pm 0.02 & 0.70 \pm 0.02 & -0.11 \\ \text{hept.l.ene} & -0.33 \pm 0.00 & 3.30 \pm 0.02 & 2.97 \pm 0.02 & 1.66 \\ \text{hept.l.yne} & -0.80 \pm 0.00 & 3.08 \pm 0.02 & 2.28 \pm 0.02 & 0.60 \\ \text{heptan.l.ol} & -5.09 \pm 0.01 & 2.37 \pm 0.02 & -2.80 \pm 0.02 & -3.04 \\ \text{heptan.4-one} & -5.30 \pm 0.01 & 2.50 \pm 0.02 & -2.80 \pm 0.02 & -3.04 \\ \text{heptan.4-one} & -5.19 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.92 \\ \text{heptanal} & -5.06 \pm 0.01 & 2.43 \pm 0.03 & -2.63 \pm 0.03 & -2.67 \\ \text{hex.1.ene} & -0.33 \pm 0.00 & 2.92 \pm 0.02 & 2.59 \pm 0.02 & 1.58 \\ \text{hex.1.yne} & -0.81 \pm 0.00 & 2.91 \pm 0.02 & 2.10 \pm 0.02 & 0.29 \\ \text{hexa.15.diene} & -0.65 \pm 0.01 & 3.09 \pm 0.02 & 2.44 \pm 0.02 & 1.01 \\ \text{hexafluoropropene} & -1.17 \pm 0.01 & 3.46 \pm 0.02 & 2.29 \pm 0.02 & -3.76 \\ \text{hexan.l.ol} & -5.08 \pm 0.01 & 2.51 \pm 0.02 & -2.63 \pm 0.03 & -2.67 \\ \text{hexan.l.ol} & -5.08 \pm 0.01 & 2.51 \pm 0.02 & -2.63 \pm 0.02 & -3.76 \\ \text{hexan.l.ol} & -5.08 \pm 0.01 & 2.05 \pm 0.02 & 2.44 \pm 0.02 & 1.01 \\ \text{hexafluoropropene} & -1.17 \pm 0.01 & 3.46 \pm 0.02 & 2.29 \pm 0.02 & -3.76 \\ \text{hexan.l.ol} & -5.09 \pm 0.01 & 2.51 \pm 0.02 & -2.77 \pm 0.02 & -3.28 \\ \text{hexan.2-one} & -5.28 \pm 0.01 & 2.51 \pm 0.02 & -2.77 \pm 0.02 & -3.28 \\ \text{hexan.3-ol} & -6.93 \pm 0.02 & 1.58 \pm 0.02 & -2.66 \pm 0.02 & -2.81 \\ \text{hexanol} & -6.93 \pm 0.02 & 1.58 \pm 0.02 & -2.69 \pm 0.02 & -2.81 \\ \text{hexanol} & -6.93 \pm 0.02 & 1.58 \pm 0.02 & -2.69 \pm 0.02 & -2.81 \\ \text{hexanol} & -6.93 \pm 0.02 & 1.58 \pm 0.02 & -2.69 \pm 0.02 & -2.81 \\ \text{hexanol} & -6.93 \pm 0.02 & 1.26 \pm 0.01 & -7.10 \pm 0.02 & -9.30 \\ \text{hydrazine} & -8.36 \pm 0.02 & 1.26 \pm 0.01 & -7.10 \pm 0.02 & -9.30 \\ \text{hydrogen.sulfide} & -3.05 \pm 0.01 & 1.88 \pm 0.01 & -1.17 \pm 0.01 & -0.7$					
$\begin{array}{c} \text{thylbenzene} & -2.76 \pm 0.01 & 2.17 \pm 0.02 & -0.59 \pm 0.02 & -0.79 \\ \text{fluorene} & -5.31 \pm 0.01 & 1.02 \pm 0.02 & -4.29 \pm 0.02 & -3.35 \\ \text{fluorobenzene} & -2.10 \pm 0.01 & 2.03 \pm 0.02 & -0.07 \pm 0.02 & -0.80 \\ \text{fluoromethane} & -1.61 \pm 0.01 & 2.40 \pm 0.01 & 0.79 \pm 0.01 & -0.22 \\ \text{formaldehyde} & -4.87 \pm 0.01 & 1.65 \pm 0.01 & -3.22 \pm 0.01 & -2.75 \\ \text{halothane} & -1.59 \pm 0.01 & 2.29 \pm 0.02 & 0.70 \pm 0.02 & -0.11 \\ \text{hept.1.ene} & -0.33 \pm 0.00 & 3.30 \pm 0.02 & 2.97 \pm 0.02 & 1.66 \\ \text{hept.1.yne} & -0.80 \pm 0.00 & 3.08 \pm 0.02 & 2.28 \pm 0.02 & 0.60 \\ \text{heptan.1.ol} & -5.09 \pm 0.01 & 2.37 \pm 0.02 & -2.72 \pm 0.02 & -4.21 \\ \text{heptan.2.one} & -5.30 \pm 0.01 & 2.50 \pm 0.02 & -2.80 \pm 0.02 & -3.04 \\ \text{heptan.4.one} & -5.19 \pm 0.01 & 2.51 \pm 0.02 & -2.68 \pm 0.02 & -2.99 \\ \text{heptan.al} & -5.06 \pm 0.01 & 2.43 \pm 0.03 & -2.63 \pm 0.03 & -2.67 \\ \text{hex.1.ene} & -0.33 \pm 0.00 & 2.92 \pm 0.02 & 2.59 \pm 0.02 & 1.58 \\ \text{hex.1.yne} & -0.81 \pm 0.00 & 2.91 \pm 0.02 & 2.10 \pm 0.02 & 0.29 \\ \text{hexa.15.diene} & -0.65 \pm 0.01 & 3.09 \pm 0.02 & 2.44 \pm 0.02 & 1.01 \\ \text{hexafluoropropene} & -1.17 \pm 0.01 & 3.46 \pm 0.02 & 2.29 \pm 0.02 & -3.76 \\ \text{hexan.1.ol} & -5.08 \pm 0.01 & 2.05 \pm 0.02 & -2.03 \pm 0.03 & -3.67 \\ \text{hexan.3.ol} & -4.96 \pm 0.01 & 2.33 \pm 0.02 & -2.63 \pm 0.02 & -3.28 \\ \text{hexan.3.ol} & -4.96 \pm 0.01 & 2.33 \pm 0.02 & -2.66 \pm 0.02 & -3.28 \\ \text{hexan.3.ol} & -4.96 \pm 0.01 & 2.33 \pm 0.02 & -2.66 \pm 0.02 & -3.28 \\ \text{hexan.al} & -5.09 \pm 0.01 & 2.13 \pm 0.02 & -2.66 \pm 0.02 & -3.28 \\ \text{hexan.al} & -5.09 \pm 0.01 & 2.13 \pm 0.02 & -2.66 \pm 0.02 & -2.81 \\ \text{hydrazine} & -8.36 \pm 0.02 & 1.26 \pm 0.01 & -7.10 \pm 0.02 & -9.30 \\ \text{hydrogen.sulfide} & -3.05 \pm 0.01 & 1.88 \pm 0.01 & -1.17 \pm 0.01 & -0.70 \\ \text{imidazole} & -8.49 \pm 0.02 & 0.64 \pm 0.02 & -7.85 \pm 0.03 & -6.21 \\ \text{hydrogen.sulfide} & -3.05 \pm 0.01 & 1.27 \pm 0.02 & -7.85 \pm 0.03 & -9.63 \\ \text{indone} & -2.97 \pm 0.01 & 1.77 \pm 0.02 & -0.34 \pm 0.02 & -1.74 \\ \text{iodobehane} & -1.90 \pm 0.01 & 1.93 \pm 0.01 & 0.03 \pm 0.01 & -0.89 \\ \end{array}$					
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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 hydrazine -8.36 ± 0.02 1.85 ± 0.02 -5.08 ± 0.03 -6.21 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 iodomethane<					
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iodomethane -1.90 ± 0.01 1.93 ± 0.01 0.03 ± 0.01 -0.89					
isoamyl_acetate $ -5.44 \pm 0.01 2.39 \pm 0.03 -3.05 \pm 0.03 -2.21 $					
	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	-5.17 ± 0.01 -5.23 ± 0.01	2.43 ± 0.02	-3.39 ± 0.02 -2.80 ± 0.02	-2.13
isobutyl_formate	-5.00 ± 0.01	1.79 ± 0.02	-3.21 ± 0.02	-2.22
isobutyl_isobutanoate	-5.29 ± 0.01	2.74 ± 0.02	$\frac{3.21 \pm 0.02}{-2.55 \pm 0.03}$	-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	$\frac{2.33 \pm 0.02}{-1.38 \pm 0.02}$	0.10
isopropyl_acetate	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-2.64
isopropyl_acetate isopropyl_formate	-3.13 ± 0.02 -4.37 ± 0.01	1.73 ± 0.02	$\frac{-2.92 \pm 0.03}{-2.64 \pm 0.02}$	-2.04
isopropylbenzene	-2.86 ± 0.01	$\frac{1.73 \pm 0.02}{2.55 \pm 0.02}$	-0.31 ± 0.02	-0.30
m_bis_trifluoromethylbenzene	-4.19 ± 0.01	2.60 ± 0.02 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 ± 0.02	-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 ± 0.02	-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 n_hexylamine	-5.49 ± 0.01	2.52 ± 0.03	$\frac{-2.97 \pm 0.03}{2.54 \pm 0.02}$	-2.26
n_nexylamine n_hexylbenzene	-4.88 ± 0.01	2.34 ± 0.02	-2.54 ± 0.02	-3.95
·	$-2.71 \pm 0.01 0.01 \pm 0.00$	$2.95 \pm 0.03 \\ 3.31 \pm 0.03$	$0.24 \pm 0.03 3.32 \pm 0.03$	-0.04 3.13
n_nonane	0.01 ± 0.00	0.01 ± 0.03	5.52 ± 0.05	3.13

n_octane	0.01 ± 0.00	3.12 ± 0.03	3.13 ± 0.03	2.88
n_octylamine	-5.12 ± 0.01	3.12 ± 0.03 2.74 ± 0.03	-2.38 ± 0.03	-3.65
n_pentane	-3.12 ± 0.01 0.01 ± 0.00	2.66 ± 0.02	$\frac{-2.38 \pm 0.03}{2.67 \pm 0.02}$	2.32
n_pentyl_acetate	-5.40 ± 0.00	2.57 ± 0.03	-2.83 ± 0.03	-2.51
n_pentyl_acetate n_pentyl_propanoate	-5.40 ± 0.01 -5.96 ± 0.01	2.60 ± 0.03	-2.83 ± 0.03 -3.36 ± 0.03	-2.31
n_pentylamine	-5.90 ± 0.01 -5.12 ± 0.01	2.00 ± 0.03 2.13 ± 0.02		-4.09
n_pentylbenzene	-3.12 ± 0.01 -2.75 ± 0.01	2.13 ± 0.02 2.80 ± 0.03	-2.99 ± 0.02 0.05 ± 0.03	-0.23
n_pentylcyclopentane	0.00 ± 0.00 -2.41 ± 0.01	2.39 ± 0.03	2.39 ± 0.03	2.55
n_propanethiol		2.10 ± 0.02 1.97 ± 0.02	-0.31 ± 0.02 -3.33 ± 0.02	-1.06
n_propyl_acetate	-5.30 ± 0.01	1.97 ± 0.02 2.47 ± 0.03		-2.79
n_propyl_butyrate	-5.35 ± 0.01		-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 1.94 ± 0.02	-3.29 ± 0.02	-3.52
pentan_3_ol	-4.89 ± 0.01		-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 1.64 ± 0.02	-1.24 ± 0.02	-3.52
pentanoic_acid	-7.01 ± 0.06		-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	ΔG_{elec} .	ΔG_{vdw} .	ΔG_{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 Open-Eye's Lexichem package).