SUPPLEMENTAL MATERIAL FOR

# ENTHALPY OF SOLVATION CORRELATIONS FOR GASEOUS SOLUTES DISSOLVED IN BENZENE AND IN ALKANE SOLVENTS BASED ON THE ABRAHAM MODEL

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TABLE S1. Values of the gas to heptane solvation enthalpy in kJ/mol at 298K for 134 solutes, together with the solute descriptors.

| Solute | **E** | **S** | **A** | **B** | **L** | **V** | Exp. Value | Ref. |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Methane | 0.000 | 0.000 | 0.000 | 0.000 | -0.323 | 0.2495 | -3.81 | 27 |
| Ethane | 0.000 | 0.000 | 0.000 | 0.000 | 0.492 | 0.3904 | -11.17 | 27 |
| Pentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.162 | 0.8131 | -26.53 | 18 |
| Hexane | 0.000 | 0.000 | 0.000 | 0.000 | 2.668 | 0.9540 | -31.55 | 18 |
| Heptane | 0.000 | 0.000 | 0.000 | 0.000 | 3.173 | 1.0949 | -36.57 | 18 |
| Octane | 0.000 | 0.000 | 0.000 | 0.000 | 3.677 | 1.2358 | -41.51 | 18 |
| Nonane | 0.000 | 0.000 | 0.000 | 0.000 | 4.182 | 1.3767 | -46.40 | 18 |
| Decane | 0.000 | 0.000 | 0.000 | 0.000 | 4.686 | 1.5176 | -51.38 | 18 |
| Dodecane | 0.000 | 0.000 | 0.000 | 0.000 | 5.696 | 1.7994 | -61.17 | 18 |
| Hexadecane | 0.000 | 0.000 | 0.000 | 0.000 | 7.714 | 2.3630 | -80.92 | 18 |
| 3-Ethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.091 | 1.0949 | -35.19 | 46 |
| 2-Methylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.503 | 0.9540 | -30.05 | 52 |
| 3-Methylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.581 | 0.9540 | -30.43 | 52 |
| 2,2-Dimethylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.352 | 0.9540 | -27.85 | 52 |
| 2,3-Dimethylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.495 | 0.9540 | -29.30 | 52 |
| 2,4-Dimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.809 | 1.0949 | -32.92 | 46 |
| 2,2,4-Trimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.106 | 1.2358 | -35.06 | 53 |
| Cyclohexane | 0.305 | 0.100 | 0.000 | 0.000 | 2.964 | 0.8454 | -32.29 | 46 |
| Cycloheptane | 0.350 | 0.100 | 0.000 | 0.000 | 3.704 | 0.9863 | -37.81 | 52 |
| Cyclooctane | 0.413 | 0.100 | 0.000 | 0.000 | 4.329 | 1.1272 | -42.66 | 52 |
| Cyclodecane | 0.474 | 0.100 | 0.000 | 0.000 | 5.340 | 1.4090 | -52.10 | 52 |
| Methylcyclopentane | 0.225 | 0.100 | 0.000 | 0.000 | 2.816 | 0.8454 | -31.39 | 52 |
| Methylcyclohexane | 0.244 | 0.100 | 0.000 | 0.000 | 3.323 | 0.9863 | -35.37 | 52 |
| cis-1,2-Dimethylcyclohexane | 0.281 | 0.240 | 0.000 | 0.000 | 3.847 | 1.1272 | -39.76 | 52 |
| trans-1,2-Dimethylcyclohexane | 0.227 | 0.200 | 0.000 | 0.000 | 3.722 | 1.1272 | -38.69 | 52 |
| cis Decalin | 0.550 | 0.250 | 0.000 | 0.000 | 5.156 | 1.3004 | -50.82 | 52 |
| trans Decalin | 0.467 | 0.230 | 0.000 | 0.000 | 4.984 | 1.3004 | -49.95 | 52 |
| Bicyclohexyl | 0.531 | 0.330 | 0.000 | 0.070 | 5.922 | 1.5822 | -57.84 | 52 |
| Tetralin | 0.891 | 0.650 | 0.000 | 0.170 | 5.203 | 1.1714 | -52.80 | 52 |
| 1-Hexene | 0.078 | 0.080 | 0.000 | 0.070 | 2.572 | 0.9110 | -30.38 | 54 |
| 1-Octyne | 0.155 | 0.220 | 0.090 | 0.100 | 3.521 | 1.1498 | -40.04 | 20 |
| 2-Octyne | 0.225 | 0.300 | 0.000 | 0.100 | 3.850 | 1.1498 | -42.63 | 20 |
| Propanal | 0.196 | 0.650 | 0.000 | 0.450 | 1.815 | 0.5470 | -20.19 | 55 |
| Butanal | 0.187 | 0.650 | 0.000 | 0.450 | 2.270 | 0.6879 | -25.19 | 55 |
| Pentanal | 0.163 | 0.650 | 0.000 | 0.450 | 2.770 | 0.8288 | -31.15 | 55 |
| Hexanal | 0.146 | 0.650 | 0.000 | 0.450 | 3.370 | 0.9697 | -36.45 | 55 |
| Heptanal | 0.140 | 0.650 | 0.000 | 0.450 | 3.860 | 1.1106 | -41.59 | 55 |
| Octanal | 0.160 | 0.650 | 0.000 | 0.450 | 4.380 | 1.2515 | -45.76 | 55 |
| Nonanal | 0.150 | 0.650 | 0.000 | 0.450 | 4.856 | 1.3924 | -50.84 | 55 |
| 2-Methylpropanal | 0.144 | 0.620 | 0.000 | 0.450 | 2.120 | 0.6879 | -26.30 | 55 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Acetone | 0.179 | 0.700 | 0.040 | 0.490 | 1.696 | 0.5470 | -21.59 | 19 |
| 2-Butanone | 0.166 | 0.700 | 0.000 | 0.510 | 2.287 | 0.6879 | -26.53 | 19 |
| 2-Heptanone | 0.123 | 0.680 | 0.000 | 0.510 | 3.760 | 1.1106 | -41.09 | 19 |
| 4-Heptanone | 0.110 | 0.660 | 0.000 | 0.510 | 3.705 | 1.1106 | -41.51 | 19 |
| 2-Nonanone | 0.119 | 0.680 | 0.000 | 0.510 | 4.735 | 1.3924 | -50.12 | 19 |
| 5-Nonanone | 0.103 | 0.660 | 0.000 | 0.510 | 4.698 | 1.3924 | -50.08 | 19 |
| 2,2,4,4-Tetramethyl-3-pentanone | 0.099 | 0.560 | 0.000 | 0.520 | 4.370 | 1.3924 | -42.13 | 19 |
| Cyclohexanone | 0.403 | 0.860 | 0.000 | 0.560 | 3.792 | 0.8610 | -37.78 | 19 |
| Butyl acetate | 0.071 | 0.600 | 0.000 | 0.450 | 3.353 | 1.0284 | -38.72 | 56 |
| Pentyl acetate | 0.067 | 0.600 | 0.000 | 0.450 | 3.844 | 1.1693 | -44.52 | 1 |
| Ethyl benzoate | 0.689 | 0.850 | 0.000 | 0.460 | 5.076 | 1.2140 | -53.08 | 5 |
| Methyl methacrylate | 0.245 | 0.510 | 0.000 | 0.440 | 2.880 | 0.8445 | -33.11 | 113 |
| Diethyl ether | 0.041 | 0.250 | 0.000 | 0.450 | 2.015 | 0.7309 | -24.31 | 16 |
| Dibutyl ether | 0.000 | 0.250 | 0.000 | 0.450 | 3.924 | 1.2950 | -44.22 | 114 |
| Dipentyl ether | 0.000 | 0.250 | 0.000 | 0.450 | 4.875 | 1.5763 | -52.54 | 57 |
| Diisopropyl ether | -0.060 | 0.160 | 0.000 | 0.580 | 2.530 | 1.0127 | -30.96 | 46 |
| Butyl methyl ether | 0.045 | 0.250 | 0.000 | 0.440 | 2.658 | 0.8718 | -30.79 | 17 |
| Methyl heptyl ether | 0.048 | 0.250 | 0.000 | 0.450 | 4.088 | 1.2945 | -46.11 | 114 |
| Methyl *tert*-butyl ether | 0.024 | 0.210 | 0.000 | 0.590 | 2.380 | 0.8718 | -24.81 | 16 |
| Ethyl *tert*-butyl ether | -0.020 | 0.160 | 0.000 | 0.600 | 2.720 | 1.0127 | -32.28 | 58 |
| Methyl *tert*-amyl ether | 0.050 | 0.210 | 0.000 | 0.600 | 2.916 | 1.0127 | -34.61 | 59 |
| Tetrahydrofuran | 0.289 | 0.520 | 0.000 | 0.480 | 2.636 | 0.6223 | -29.32 | 61 |
| 2-Methyltetrahydrofuran | 0.241 | 0.480 | 0.000 | 0.530 | 2.820 | 0.7632 | -31.59 | 60 |
| 2,5,8,11,14-Pentaoxopentadecane | -0.020 | 1.110 | 0.000 | 1.790 | 6.498 | 1.8111 | -68.10 | 2 |
| 2,5,8,11-Tetraoxododecane | 0.000 | 0.980 | 0.000 | 1.440 | 5.157 | 1.4706 | -54.121 | 6 |
| 2,5,8-Trioxanonane | 0.113 | 0.760 | 0.000 | 1.170 | 3.920 | 1.1301 | -39.94 | 7 |
| Diethoxymethane | 0.010 | 0.490 | 0.000 | 0.540 | 2.789 | 0.9305 | -33.14 | 3 |
| 1,2-Dimethoxyethane | 0.116 | 0.670 | 0.000 | 0.680 | 2.654 | 0.7896 | -31.76 | 3 |
| Dimethoxymethane | 0.099 | 0.460 | 0.000 | 0.520 | 1.894 | 0.6487 | -26.06 | 3 |
| 1-Fluorooctane | -0.020 | 0.350 | 0.000 | 0.100 | 3.850 | 1.2538 | -47.86 | 114 |
| Tetrachloromethane | 0.458 | 0.380 | 0.000 | 0.000 | 2.823 | 0.7391 | -31.21 | 110 |
| 1,2-Dichloroethane | 0.416 | 0.640 | 0.100 | 0.110 | 2.573 | 0.6352 | -27.98 | 62 |
| 1-Chlorooctane | 0.191 | 0.400 | 0.000 | 0.090 | 4.708 | 1.3585 | -50.88 | 114 |
| Diiodomethane | 0.714 | 0.690 | 0.110 | 0.070 | 2.886 | 0.7659 | -37.74 | 110 |
| Methanol | 0.278 | 0.440 | 0.430 | 0.470 | 0.970 | 0.3082 | -14.90 | 63 |
| Ethanol | 0.246 | 0.420 | 0.370 | 0.480 | 1.485 | 0.4491 | -18.60 | 63 |
| 1-Propanol | 0.236 | 0.420 | 0.370 | 0.480 | 2.031 | 0.5900 | -22.10 | 8 |
| Butan-1-ol | 0.224 | 0.420 | 0.370 | 0.480 | 2.601 | 0.7309 | -27.87 | 16 |
| Pentan-1-ol | 0.219 | 0.420 | 0.370 | 0.480 | 3.106 | 0.8718 | -34.14 | 16 |
| 1-Hexanol | 0.210 | 0.420 | 0.370 | 0.480 | 3.610 | 1.0170 | -38.32 | 8 |
| 1-Octanol | 0.199 | 0.420 | 0.370 | 0.480 | 4.619 | 1.2950 | -47.57 | 114 |
| 1-Nonanol | 0.193 | 0.420 | 0.370 | 0.480 | 5.124 | 1.4354 | -53.66 | 64 |
| 1-Undecanol | 0.181 | 0.420 | 0.370 | 0.480 | 6.130 | 1.7173 | -61.83 | 64 |
| 2-Butanol | 0.217 | 0.360 | 0.330 | 0.560 | 2.338 | 0.7309 | -26.70 | 9 |
| 2-Methyl-1-propanol | 0.217 | 0.390 | 0.370 | 0.480 | 2.413 | 0.7309 | -26.60 | 9 |
| 2-Methyl-2-propanol | 0.180 | 0.300 | 0.310 | 0.600 | 1.963 | 0.7309 | -22.60 | 9 |
| 3-Methyl-1-butanol | 0.192 | 0.390 | 0.370 | 0.480 | 3.011 | 0.8718 | -35.63 | 65 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 2-Pentanol | 0.195 | 0.360 | 0.330 | 0.560 | 2.840 | 0.8718 | -35.90 | 65 |
| 3-Methyl-2-butanol | 0.194 | 0.330 | 0.330 | 0.560 | 2.793 | 0.8718 | -31.93 | 65 |
| 2-Methyl-2-butanol | 0.194 | 0.300 | 0.310 | 0.600 | 2.630 | 0.8718 | -26.44 | 16 |
| Cyclopentanol | 0.427 | 0.540 | 0.320 | 0.560 | 3.241 | 0.7630 | -37.21 | 10 |
| Cyclohexanol | 0.460 | 0.540 | 0.320 | 0.570 | 3.758 | 0.9040 | -37.50 | 66 |
| 2-Methoxyethanol | 0.269 | 0.500 | 0.300 | 0.840 | 2.490 | 0.6487 | -34.22 | 68 |
| Triethylamine | 0.101 | 0.150 | 0.000 | 0.790 | 3.040 | 1.0538 | -34.45 | 46 |
| Propylamine | 0.225 | 0.350 | 0.160 | 0.610 | 2.141 | 0.6311 | -25.14 | 66 |
| Isopropylamine | 0.181 | 0.320 | 0.160 | 0.610 | 1.908 | 0.6311 | -22.87 | 66 |
| Butylamine | 0.224 | 0.350 | 0.160 | 0.610 | 2.618 | 0.7720 | -29.97 | 66 |
| sec-Butylamine | 0.170 | 0.320 | 0.160 | 0.630 | 2.410 | 0.7720 | -27.89 | 66 |
| iso-Butylamine | 0.121 | 0.290 | 0.160 | 0.710 | 2.493 | 0.7720 | -28.11 | 66 |
| *tert*-Butylamine | 0.121 | 0.290 | 0.160 | 0.710 | 2.493 | 0.7720 | -24.98 | 66 |
| Pentylamine | 0.211 | 0.350 | 0.160 | 0.610 | 3.139 | 0.9129 | -34.12 | 66 |
| Hexylamine | 0.197 | 0.350 | 0.160 | 0.610 | 3.655 | 1.0538 | -39.47 | 66 |
| Heptylamine | 0.197 | 0.350 | 0.160 | 0.610 | 4.153 | 1.1947 | -44.97 | 66 |
| Octylamine | 0.187 | 0.350 | 0.160 | 0.610 | 4.520 | 1.3350 | -49.41 | 66 |
| Nonylamine | 0.187 | 0.350 | 0.160 | 0.610 | 5.100 | 1.4765 | -54.09 | 66 |
| Decylamine | 0.182 | 0.350 | 0.160 | 0.610 | 5.606 | 1.6174 | -58.69 | 66 |
| 3-Methylphenol | 0.822 | 0.880 | 0.570 | 0.340 | 4.310 | 0.9160 | -39.92 | 16 |
| Benzene | 0.610 | 0.520 | 0.000 | 0.140 | 2.786 | 0.7176 | -30.54 | 17 |
| Toluene | 0.601 | 0.520 | 0.000 | 0.140 | 3.325 | 0.8573 | -35.94 | 17 |
| Mesitylene | 0.649 | 0.520 | 0.000 | 0.190 | 4.344 | 1.1391 | -46.23 | 17 |
| Naphthalene | 1.340 | 0.920 | 0.000 | 0.200 | 5.161 | 1.0854 | -51.82 | 69 |
| Trifluorotoluene | 0.225 | 0.480 | 0.000 | 0.100 | 2.894 | 0.9104 | -33.35 | 17 |
| Nitrobenzene | 0.871 | 1.110 | 0.000 | 0.280 | 4.557 | 0.8906 | -44.73 | 17 |
| Anisole | 0.710 | 0.750 | 0.000 | 0.290 | 3.890 | 0.9160 | -41.21 | 17 |
| Aniline | 0.955 | 0.960 | 0.260 | 0.410 | 3.934 | 0.8162 | -40.75 | 15 |
| Acetonitrile | 0.237 | 0.900 | 0.070 | 0.320 | 1.739 | 0.4042 | -17.56 | 70 |
| Helium | 0.000 | 0.000 | 0.000 | 0.000 | -1.741 | 0.0608 | 7.72 | 27 |
| Neon | 0.000 | 0.000 | 0.000 | 0.000 | -1.575 | 0.0850 | 5.56 | 27 |
| Argon | 0.000 | 0.000 | 0.000 | 0.000 | -0.688 | 0.1900 | -1.22 | 27 |
| Krypton | 0.000 | 0.000 | 0.000 | 0.000 | -0.211 | 0.2460 | -5.51 | 27 |
| Xenon | 0.000 | 0.000 | 0.000 | 0.000 | 0.378 | 0.3290 | -10.08 | 71 |
| Hydrogen | 0.000 | 0.000 | 0.000 | 0.000 | -1.200 | 0.1086 | 3.78 | 27 |
| Carbon dioxide | 0.000 | 0.280 | 0.050 | 0.100 | 0.058 | 0.2809 | -9.66 | 27 |
| Tetrafluoromethane | -0.580 | -0.260 | 0.000 | 0.000 | -0.817 | 0.3202 | -1.59 | 27 |
| Sulfur hexafluoride | -0.600 | -0.200 | 0.000 | 0.000 | -0.120 | 0.4643 | -8.28 | 27 |
| Sulfur dioxide | 0.370 | 0.660 | 0.280 | 0.100 | 0.778 | 0.3465 | -15.90 | 4 |
| Difluorodichloromethane | 0.037 | 0.130 | 0.000 | 0.000 | 1.124 | 0.5297 | -18.91 | 27 |
| Hexafluorobenzene | 0.088 | 0.560 | 0.000 | 0.010 | 2.345 | 0.8226 | -31.62 | 72 |
| Chlorotrifluoromethane | -0.247 | -0.046 | 0.000 | 0.000 | 0.209 | 0.4250 | -12.84 | 27 |
| Nitromethane | 0.313 | 0.950 | 0.060 | 0.310 | 1.892 | 0.4237 | -24.40 | 74 |
| 1-Methylnaphthalene | 1.337 | 0.940 | 0.000 | 0.220 | 5.802 | 1.2260 | -54.06 | 73 |
| 1-Butanethiol | 0.382 | 0.350 | 0.000 | 0.240 | 3.243 | 0.8357 | -33.81 | 42 |
| 1,2,4-Trimethylbenzene | 0.677 | 0.560 | 0.000 | 0.190 | 4.441 | 1.1391 | -46.76 | 115 |

TABLE S2. Values of the gas to hexadecane solvation enthalpy in kJ/mol at 298K for 102 solutes, together with the solute descriptors.

| Solute | E | S | A | B | L | V | Exp Value | Ref. |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Methane | 0.000 | 0.000 | 0.000 | 0.000 | -0.323 | 0.2945 | -3.97 | 12 |
| Ethane | 0.000 | 0.000 | 0.000 | 0.000 | 0.492 | 0.3904 | -11.51 | 12 |
| Propane | 0.000 | 0.000 | 0.000 | 0.000 | 1.050 | 0.5313 | -15.94 | 12 |
| Butane | 0.000 | 0.000 | 0.000 | 0.000 | 1.615 | 0.6722 | -20.79 | 12 |
| Pentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.162 | 0.8131 | -25.94 | 12 |
| Hexane | 0.000 | 0.000 | 0.000 | 0.000 | 2.668 | 0.9540 | -31.04 | 12 |
| Heptane | 0.000 | 0.000 | 0.000 | 0.000 | 3.173 | 1.0949 | -36.15 | 12 |
| Octane | 0.000 | 0.000 | 0.000 | 0.000 | 3.677 | 1.2358 | -41.13 | 12 |
| Hexadecane | 0.000 | 0.000 | 0.000 | 0.000 | 7.714 | 2.3630 | -81.38 | 12 |
| 2-Methylpropane | 0.000 | 0.000 | 0.000 | 0.000 | 1.409 | 0.6722 | -18.74 | 12 |
| 2,2-Dimethylpropane | 0.000 | 0.000 | 0.000 | 0.000 | 1.820 | 0.8131 | -21.14 | 112 |
| Cyclopentane | 0.263 | 0.100 | 0.000 | 0.000 | 2.477 | 0.7045 | -27.66 | 12 |
| Cyclohexane | 0.305 | 0.100 | 0.000 | 0.000 | 2.964 | 0.8454 | -31.50 | 12 |
| Ethene | 0.107 | 0.100 | 0.000 | 0.070 | 0.289 | 0.3474 | -11.17 | 12 |
| Propene | 0.103 | 0.080 | 0.000 | 0.070 | 0.946 | 0.4883 | -13.35 | 12 |
| Acetone | 0.179 | 0.700 | 0.040 | 0.490 | 1.696 | 0.5470 | -21.42 | 12 |
| 2-Butanone | 0.166 | 0.700 | 0.000 | 0.510 | 2.287 | 0.6879 | -26.48 | 12 |
| 2-Pentanone | 0.143 | 0.680 | 0.000 | 0.510 | 2.755 | 0.8288 | -31.05 | 12 |
| 2-Hexanone | 0.136 | 0.680 | 0.000 | 0.510 | 3.286 | 0.9697 | -35.77 | 12 |
| 2-Heptanone | 0.123 | 0.680 | 0.000 | 0.510 | 3.760 | 1.1106 | -40.46 | 12 |
| 4-Heptanone | 0.110 | 0.660 | 0.000 | 0.510 | 3.705 | 1.1106 | -44.89 | 12 |
| 2-Octanone | 0.108 | 0.680 | 0.000 | 0.510 | 4.257 | 1.2515 | -44.89 | 12 |
| 2-Nonanone | 0.119 | 0.680 | 0.000 | 0.510 | 4.735 | 1.3924 | -49.37 | 12 |
| Cyclohexanone | 0.403 | 0.860 | 0.000 | 0.560 | 3.792 | 0.8610 | -36.48 | 12 |
| Diethyl ether | 0.041 | 0.250 | 0.000 | 0.450 | 2.015 | 0.7309 | -25.19 | 12 |
| Dipropyl ether | 0.008 | 0.250 | 0.000 | 0.450 | 2.954 | 1.0127 | -34.15 | 75 |
| Dibutyl ether | 0.000 | 0.250 | 0.000 | 0.450 | 3.924 | 1.2950 | -43.42 | 76 |
| Butyl methyl ether | 0.045 | 0.250 | 0.000 | 0.440 | 2.658 | 0.8718 | -30.53 | 77 |
| Diisopropyl ether | -0.060 | 0.160 | 0.000 | 0.580 | 2.530 | 1.0170 | -30.67 | 107 |
| Methyl *tert*-amyl ether | 0.050 | 0.210 | 0.000 | 0.600 | 2.916 | 1.0170 | -34.12 | 106 |
| Tetrahydrofuran | 0.289 | 0.520 | 0.000 | 0.480 | 2.636 | 0.6223 | -28.53 | 12 |
| 2-Methyltetrahydrofuran | 0.241 | 0.480 | 0.000 | 0.530 | 2.820 | 0.7632 | -30.78 | 78 |
| Dichloromethane | 0.387 | 0.570 | 0.100 | 0.050 | 2.019 | 0.4643 | -23.18 | 12 |
| Chloroform | 0.425 | 0.490 | 0.150 | 0.020 | 2.480 | 0.6167 | -28.07 | 12 |
| Carbon tetrachloride | 0.458 | 0.380 | 0.000 | 0.000 | 2.823 | 0.7391 | -30.92 | 12 |
| 1-Chlorobutane | 0.210 | 0.400 | 0.000 | 0.100 | 2.722 | 0.7946 | -30.88 | 12 |
| Tetrachloroethene | 0.639 | 0.440 | 0.000 | 0.000 | 3.584 | 0.8370 | -38.41 | 12 |
| Nitromethane | 0.313 | 0.950 | 0.060 | 0.310 | 1.892 | 0.4237 | -25.36 | 12 |
| 2-Nitropropane | 0.216 | 0.920 | 0.000 | 0.330 | 2.550 | 0.7055 | -30.15 | 39 |
| Acetonitrile | 0.237 | 0.900 | 0.070 | 0.320 | 1.739 | 0.4042 | -19.08 | 12 |
| Methanol | 0.278 | 0.440 | 0.430 | 0.470 | 0.970 | 0.3082 | -13.35 | 12 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Ethanol | 0.246 | 0.420 | 0.370 | 0.480 | 1.485 | 0.4491 | -16.32 | 12 |
| 1-Propanol | 0.236 | 0.420 | 0.370 | 0.480 | 2.031 | 0.5900 | -21.17 | 12 |
| 2-Propanol | 0.212 | 0.360 | 0.330 | 0.560 | 1.764 | 0.5900 | -22.38 | 12 |
| 1-Butanol | 0.224 | 0.420 | 0.370 | 0.480 | 2.601 | 0.7309 | -28.07 | 12 |
| 1-Pentanol | 0.219 | 0.420 | 0.370 | 0.480 | 3.106 | 0.8718 | -31.34 | 12 |
| 1-Hexanol | 0.210 | 0.420 | 0.370 | 0.480 | 3.610 | 1.0170 | -39.79 | 12 |
| Heptan-1-ol | 0.211 | 0.420 | 0.370 | 0.480 | 4.115 | 1.1536 | -44.43 | 12 |
| 1-Octanol | 0.199 | 0.420 | 0.370 | 0.480 | 4.619 | 1.2950 | -49.07 | 12 |
| 1-Nonanol | 0.193 | 0.420 | 0.370 | 0.480 | 5.124 | 1.4354 | -52.81 | 64 |
| 1-Undecanol | 0.181 | 0.420 | 0.370 | 0.480 | 6.130 | 1.7173 | -61.39 | 64 |
| tert-Butanol | 0.180 | 0.300 | 0.310 | 0.600 | 1.963 | 0.7309 | -23.01 | 12 |
| Cyclohexanol | 0.460 | 0.540 | 0.320 | 0.570 | 3.758 | 0.9040 | -47.53 | 79 |
| Ethyl acetate | 0.106 | 0.620 | 0.000 | 0.450 | 2.314 | 0.7466 | -27.99 | 12 |
| Butyl acetate | 0.071 | 0.600 | 0.000 | 0.450 | 3.353 | 1.0284 | -38.49 | 12 |
| Methyl benzoate | 0.733 | 0.850 | 0.000 | 0.460 | 4.704 | 1.0730 | -48.37 | 12 |
| Benzene | 0.610 | 0.520 | 0.000 | 0.140 | 2.786 | 0.7176 | -30.38 | 12 |
| Toluene | 0.601 | 0.520 | 0.000 | 0.140 | 3.325 | 0.8573 | -35.90 | 12 |
| Ethylbenzene | 0.613 | 0.510 | 0.000 | 0.150 | 3.778 | 0.9982 | -40.12 | 12 |
| Propylbenzene | 0.604 | 0.500 | 0.000 | 0.150 | 4.230 | 1.1391 | -44.14 | 12 |
| m-Xylene | 0.623 | 0.520 | 0.000 | 0.160 | 3.839 | 0.9982 | -41.37 | 12 |
| p-Xylene | 0.613 | 0.520 | 0.000 | 0.160 | 3.839 | 0.9982 | -41.51 | 12 |
| Mesitylene | 0.649 | 0.520 | 0.000 | 0.190 | 4.344 | 1.1391 | -46.56 | 12 |
| Acetophenone | 0.818 | 1.010 | 0.000 | 0.480 | 4.501 | 1.0140 | -47.36 | 12 |
| Anisole | 0.710 | 0.750 | 0.000 | 0.290 | 3.890 | 0.9160 | -41.24 | 12 |
| Benzaldehyde | 0.820 | 1.000 | 0.000 | 0.390 | 4.008 | 0.8730 | -41.17 | 12 |
| Benzonitrile | 0.742 | 1.110 | 0.000 | 0.330 | 4.039 | 0.8710 | -41.25 | 12 |
| Chlorobenzene | 0.718 | 0.650 | 0.000 | 0.070 | 3.657 | 0.8388 | -38.24 | 12 |
| Fluorobenzene | 0.477 | 0.570 | 0.000 | 0.100 | 2.788 | 0.7341 | -31.05 | 12 |
| 1,4-Difluorobenzene | 0.384 | 0.600 | 0.000 | 0.060 | 2.766 | 0.7518 | -32.19 | 72 |
| Aniline | 0.955 | 0.960 | 0.260 | 0.410 | 3.934 | 0.8162 | -41.80 | 12 |
| Nitrobenzene | 0.871 | 1.110 | 0.000 | 0.280 | 4.557 | 0.8906 | -45.65 | 12 |
| N,N-Dimethylaniline | 0.957 | 0.810 | 0.000 | 0.410 | 4.701 | 1.0980 | -48.36 | 12 |
| Pyridine | 0.631 | 0.840 | 0.000 | 0.520 | 3.022 | 0.6753 | -32.64 | 12 |
| 2-Methylpyridine | 0.598 | 0.750 | 0.000 | 0.580 | 3.422 | 0.8162 | -35.90 | 12 |
| 3-Methylpyridine | 0.631 | 0.810 | 0.000 | 0.540 | 3.631 | 0.8162 | -37.49 | 12 |
| 4-Methylpyridine | 0.63 | 0.820 | 0.000 | 0.540 | 3.64 | 0.8162 | -36.78 | 12 |
| Propylamine | 0.225 | 0.350 | 0.160 | 0.610 | 2.141 | 0.6311 | -23.97 | 12 |
| Butylamine | 0.224 | 0.350 | 0.160 | 0.610 | 2.618 | 0.7720 | -29.41 | 12 |
| Pentylamine | 0.211 | 0.350 | 0.160 | 0.610 | 3.139 | 0.9130 | -34.81 | 80 |
| Hexylamine | 0.197 | 0.350 | 0.160 | 0.610 | 3.655 | 1.0538 | -39.46 | 12 |
| Heptylamine | 0.197 | 0.350 | 0.160 | 0.610 | 4.153 | 1.1947 | -45.27 | 80 |
| Nonylamine | 0.187 | 0.350 | 0.160 | 0.610 | 5.100 | 1.4765 | -55.03 | 80 |
| Decylamine | 0.182 | 0.350 | 0.160 | 0.610 | 5.605 | 1.6174 | -60.02 | 80 |
| *tert*-Butylamine | 0.121 | 0.290 | 0.160 | 0.710 | 2.493 | 0.7720 | -26.15 | 12 |
| Diethylamine | 0.154 | 0.300 | 0.080 | 0.690 | 2.395 | 0.7720 | -24.60 | 12 |
| Triethylamine | 0.101 | 0.150 | 0.000 | 0.790 | 3.040 | 1.0538 | -34.14 | 12 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Helium | 0.000 | 0.000 | 0.000 | 0.000 | -1.741 | 0.0680 | 8.24 | 12 |
| Neon | 0.000 | 0.000 | 0.000 | 0.000 | -1.575 | 0.0850 | 6.78 | 12 |
| Argon | 0.000 | 0.000 | 0.000 | 0.000 | -0.688 | 0.1900 | -0.79 | 12 |
| Krypton | 0.000 | 0.000 | 0.000 | 0.000 | -0.211 | 0.2460 | -5.02 | 12 |
| Xenon | 0.000 | 0.000 | 0.000 | 0.000 | 0.378 | 0.3290 | -10.08 | 12 |
| Radon | 0.000 | 0.000 | 0.000 | 0.000 | 0.877 | 0.3840 | -14.18 | 12 |
| Hydrogen | 0.000 | 0.000 | 0.000 | 0.000 | -1.200 | 0.1086 | 4.56 | 35 |
| Diiodomethane | 0.714 | 0.690 | 0.110 | 0.070 | 2.886 | 0.7659 | -38.95 | 12 |
| 2,2,2-Trifluoroethanol | 0.015 | 0.600 | 0.570 | 0.250 | 1.224 | 0.5022 | -20.88 | 12 |
| 1,1,1,3,3,3-Hexafluoropropan-2-ol | -0.240 | 0.550 | 0.770 | 0.100 | 1.392 | 0.6962 | -22.09 | 12 |
| Benzyl alcohol | 0.803 | 0.870 | 0.330 | 0.560 | 4.221 | 0.9160 | -42.38 | 12 |
| Thiophene | 0.687 | 0.560 | 0.000 | 0.150 | 2.819 | 0.6410 | -29.92 | 12 |
| Benzyl chloride | 0.821 | 0.820 | 0.000 | 0.330 | 4.384 | 0.9797 | -43.32 | 12 |
| 1-Chloronaphthalene | 1.417 | 1.000 | 0.000 | 0.140 | 5.856 | 1.2078 | -61.74 | 82 |
| 1-Methylnaphthalene | 1.337 | 0.940 | 0.000 | 0.220 | 5.802 | 1.2260 | -55.8 | 83 |

TABLE S3. Values of the gas to cyclohexane solvation enthalpy in kJ/mol at 298K for 201 solutes, together with the solute descriptors.

| Solute | **E** | **S** | **A** | **B** | **L** | **V** | Exp. Value | Ref. |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Methane | 0.000 | 0.000 | 0.000 | 0.000 | -0.323 | 0.2495 | -3.01 | 35 |
| Ethane | 0.000 | 0.000 | 0.000 | 0.000 | 0.492 | 0.3904 | -11.13 | 35 |
| Propane | 0.000 | 0.000 | 0.000 | 0.000 | 1.050 | 0.5313 | -16.50 | 35 |
| Pentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.162 | 0.8131 | -25.52 | 18 |
| Hexane | 0.000 | 0.000 | 0.000 | 0.000 | 2.668 | 0.9540 | -30.42 | 18 |
| Heptane | 0.000 | 0.000 | 0.000 | 0.000 | 3.173 | 1.0949 | -34.94 | 18 |
| Octane | 0.000 | 0.000 | 0.000 | 0.000 | 3.677 | 1.2358 | -39.66 | 18 |
| Nonane | 0.000 | 0.000 | 0.000 | 0.000 | 4.182 | 1.3767 | -44.48 | 18 |
| Decane | 0.000 | 0.000 | 0.000 | 0.000 | 4.686 | 1.5176 | -49.08 | 18 |
| Dodecane | 0.000 | 0.000 | 0.000 | 0.000 | 5.696 | 1.7994 | -58.41 | 18 |
| Tetradecane | 0.000 | 0.000 | 0.000 | 0.000 | 6.705 | 2.0810 | -68.20 | 48 |
| Hexadecane | 0.000 | 0.000 | 0.000 | 0.000 | 7.714 | 2.3630 | -77.32 | 18 |
| 2-Methylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.013 | 0.8130 | -24.60 | 13 |
| 2,2-Dimethylpropane | 0.000 | 0.000 | 0.000 | 0.000 | 1.820 | 0.8131 | -24.27 | 48 |
| 3-Ethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.091 | 1.0949 | -34.27 | 13 |
| 2,2-Dimethylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.352 | 0.9540 | -27.16 | 13 |
| 2-Methylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.503 | 0.9540 | -28.91 | 21 |
| 3-Methylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.581 | 0.9540 | -28.87 | 48 |
| 2,2-Dimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.796 | 1.0949 | -31.38 | 48 |
| 2,3-Dimethylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.495 | 0.9540 | -27.17 | 21 |
| 2,4-Dimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.809 | 1.0949 | -31.76 | 46 |
| 3,3-Diethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.820 | 1.3767 | -41.76 | 24 |
| 3-Methylheptane | 0.000 | 0.000 | 0.000 | 0.000 | 3.510 | 1.2358 | -37.66 | 48 |
| 2-Methyloctane | 0.000 | 0.000 | 0.000 | 0.000 | 3.966 | 1.3767 | -43.10 | 48 |
| 2,2,4-Trimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.106 | 1.2358 | -34.31 | 48 |
| 2,2-Dimethylhexane | 0.000 | 0.000 | 0.000 | 0.000 | | 1.2358 | -35.56 | 48 |
| 2,2,4,4-Tetramethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.512 | 1.3767 | -38.24 | 13 |
| 2,2,5,5-Tetramethylhexane | 0.000 | 0.000 | 0.000 | 0.000 | 4.039 | 1.5176 | -40.17 | 48 |
| Cyclopentane | 0.263 | 0.100 | 0.000 | 0.000 | 2.477 | 0.7045 | -28.54 | 24 |
| Cyclohexane | 0.305 | 0.100 | 0.000 | 0.000 | 2.964 | 0.8454 | -33.05 | 13 |
| Cycloheptane | 0.350 | 0.100 | 0.000 | 0.000 | 3.704 | 0.9863 | -38.50 | 22 |
| Cyclooctane | 0.413 | 0.100 | 0.000 | 0.000 | 4.329 | 1.1272 | -43.47 | 24 |
| Methylcyclohexane | 0.244 | 0.060 | 0.000 | 0.000 | 3.319 | 0.9863 | -35.40 | 24 |
| *cis*-1,2-Dimethylcyclohexane | 0.281 | 0.240 | 0.000 | 0.000 | 3.847 | 1.1272 | -38.03 | 24 |
| Ethene | 0.107 | 0.100 | 0.000 | 0.070 | 0.289 | 0.3474 | -9.03 | 23 |
| 1-Pentene | 0.093 | 0.080 | 0.000 | 0.070 | 2.047 | 0.7701 | -24.31 | 24 |
| 1-Hexene | 0.078 | 0.080 | 0.000 | 0.070 | 2.572 | 0.9110 | -29.39 | 50 |
| 1-Heptene | 0.092 | 0.080 | 0.000 | 0.070 | 3.063 | 1.0519 | -34.18 | 24 |
| 1-Octene | 0.094 | 0.080 | 0.000 | 0.070 | 3.568 | 1.1928 | -38.95 | 24 |
| 1-Nonene | 0.090 | 0.080 | 0.000 | 0.070 | 4.073 | 1.3337 | -43.72 | 24 |
| 1-Decene | 0.090 | 0.080 | 0.000 | 0.070 | 4.554 | 1.4746 | -48.41 | 24 |

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|---|---|---|---|---|---|---|---|---|
| 1-Dodecene | 0.089 | 0.080 | 0.000 | 0.070 | 5.515 | 1.7564 | -58.24 | 24 |
| 1-Tridecene | 0.087 | 0.080 | 0.000 | 0.070 | 6.020 | 1.8973 | -63.39 | 24 |
| 1-Tetradecene | 0.085 | 0.080 | 0.000 | 0.070 | 6.513 | 2.0382 | -68.07 | 24 |
| 1-Pentadecene | 0.083 | 0.080 | 0.000 | 0.070 | 7.006 | 2.1791 | -72.97 | 24 |
| *cis* 2-Octene | 0.135 | 0.080 | 0.000 | 0.070 | 3.683 | 1.1928 | -38.16 | 24 |
| *trans* 2-Octene | 0.123 | 0.080 | 0.000 | 0.070 | 3.600 | 1.1928 | -38.24 | 24 |
| *cis* 4-Octene | 0.133 | 0.080 | 0.000 | 0.070 | 3.607 | 1.1928 | -37.99 | 24 |
| *trans* 4-Octene | 0.144 | 0.080 | 0.000 | 0.070 | 3.593 | 1.1928 | -37.70 | 24 |
| 1,5-Hexadiene | 0.191 | 0.150 | 0.000 | 0.100 | 2.450 | 0.8680 | -29.37 | 24 |
| Cyclopentene | 0.335 | 0.200 | 0.000 | 0.100 | 2.402 | 0.6605 | -27.20 | 24 |
| Cyclohexene | 0.395 | 0.200 | 0.000 | 0.100 | 3.021 | 0.8025 | -33.05 | 24 |
| 1-Methylcyclohexene | 0.391 | 0.200 | 0.000 | 0.100 | 3.483 | 0.9433 | -37.95 | 24 |
| Norbornadiene | 0.495 | 0.320 | 0.000 | 0.110 | 3.108 | 0.7919 | -33.56 | 25 |
| 1-Octyne | 0.155 | 0.220 | 0.090 | 0.100 | 3.521 | 1.1498 | -38.57 | 20 |
| 2-Octyne | 0.225 | 0.300 | 0.000 | 0.100 | 3.850 | 1.1498 | -41.59 | 20 |
| Dichloromethane | 0.387 | 0.570 | 0.100 | 0.050 | 2.019 | 0.4943 | -25.25 | 26 |
| Trichloromethane | 0.425 | 0.490 | 0.150 | 0.020 | 2.480 | 0.6167 | -28.23 | 26 |
| Tetrachloromethane | 0.458 | 0.380 | 0.000 | 0.000 | 2.823 | 0.7391 | -31.80 | 26 |
| 1-Chloropropane | 0.216 | 0.400 | 0.000 | 0.100 | 2.202 | 0.6537 | -25.42 | 26 |
| 1-Chlorobutane | 0.210 | 0.400 | 0.000 | 0.100 | 2.722 | 0.7946 | -30.62 | 13 |
| 1-Chlorooctane | 0.191 | 0.400 | 0.000 | 0.100 | 4.772 | 1.3580 | -51.46 | 13 |
| Difluorodichloromethane | 0.037 | 0.040 | 0.000 | 0.040 | 0.998 | 0.5297 | -19.75 | 28 |
| Chlorotrifluoromethane | -0.247 | -0.046 | 0.000 | 0.000 | 0.209 | 0.4250 | -9.29 | 27 |
| Diiodomethane | 1.200 | 0.690 | 0.050 | 0.170 | 3.857 | 0.7659 | -38.58 | 110 |
| Acetone | 0.179 | 0.700 | 0.040 | 0.490 | 1.696 | 0.5470 | -21.09 | 13 |
| 2-Butanone | 0.166 | 0.700 | 0.000 | 0.510 | 2.287 | 0.6879 | -26.69 | 13 |
| 2-Pentanone | 0.143 | 0.680 | 0.000 | 0.510 | 2.755 | 0.8288 | -31.30 | 13 |
| 3-Pentanone | 0.154 | 0.660 | 0.000 | 0.510 | 2.811 | 0.8288 | -30.42 | 29 |
| 2-Hexanone | 0.136 | 0.680 | 0.000 | 0.510 | 3.286 | 0.9697 | -36.15 | 13 |
| 3-Hexanone | 0.136 | 0.660 | 0.000 | 0.510 | 3.310 | 0.9697 | -34.52 | 29 |
| 2-Heptanone | 0.123 | 0.680 | 0.000 | 0.510 | 3.760 | 1.1106 | -40.67 | 13 |
| 4-Heptanone | 0.110 | 0.660 | 0.000 | 0.510 | 3.705 | 1.1106 | -39.62 | 13 |
| 2-Octanone | 0.108 | 0.680 | 0.000 | 0.510 | 4.257 | 1.2515 | -45.00 | 13 |
| 2-Nonanone | 0.119 | 0.680 | 0.000 | 0.510 | 4.735 | 1.3924 | -50.01 | 13 |
| 5-Nonanone | 0.103 | 0.660 | 0.000 | 0.510 | 4.698 | 1.3924 | -48.89 | 13 |
| 2-Decanone | 0.108 | 0.680 | 0.000 | 0.510 | 5.245 | 1.5332 | -52.51 | 29 |
| 2-Undecanone | 0.101 | 0.680 | 0.000 | 0.510 | 5.732 | 1.6740 | -56.90 | 29 |
| 6-Undecanone | 0.083 | 0.660 | 0.000 | 0.510 | 5.677 | 1.6740 | -56.27 | 29 |
| 3,3-Dimethyl-2-butanone | 0.106 | 0.620 | 0.000 | 0.510 | 2.928 | 0.9676 | -31.05 | 29 |
| 2,2,4,4-Tetramethyl-3-pentanone | 0.099 | 0.560 | 0.000 | 0.520 | 4.370 | 1.3924 | -41.05 | 116 |
| Cyclopentanone | 0.373 | 0.860 | 0.000 | 0.520 | 3.221 | 0.7200 | -33.64 | 13 |
| Cyclohexanone | 0.403 | 0.860 | 0.000 | 0.560 | 3.792 | 0.8610 | -37.65 | 13 |
| Cycloheptanone | 0.436 | 0.860 | 0.000 | 0.560 | 4.376 | 1.0020 | -42.43 | 29 |
| 2,4-Pentanedione | 0.412 | 0.780 | 0.000 | 0.630 | 3.330 | 0.8445 | -33.35 | 13 |
| Diethyl ether | 0.041 | 0.250 | 0.000 | 0.450 | 2.015 | 0.7309 | -23.05 | 16 |
| Dipropyl ether | 0.008 | 0.250 | 0.000 | 0.450 | 2.954 | 1.0127 | -34.11 | 46 |
| Diisopropyl ether | -0.060 | 0.160 | 0.000 | 0.580 | 2.530 | 1.0127 | -30.34 | 46 |

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|---|---|---|---|---|---|---|---|---|
| Methyl *tert*-butyl ether | 0.024 | 0.110 | 0.000 | 0.630 | 2.380 | 0.8718 | -28.44 | 30 |
| Ethyl *tert*-butyl ether | -0.020 | 0.160 | 0.000 | 0.600 | 2.720 | 1.0127 | -32.14 | 51 |
| Tetrahydrofuran | 0.289 | 0.520 | 0.000 | 0.480 | 2.636 | 0.6223 | -28.70 | 32 |
| Tetrahydropyran | 0.275 | 0.470 | 0.000 | 0.550 | 3.057 | 0.7672 | -33.60 | 32 |
| Butyl methyl ether | 0.045 | 0.250 | 0.000 | 0.440 | 2.658 | 0.8718 | -29.67 | 16 |
| 1,3-Dioxane | 0.308 | 0.720 | 0.000 | 0.700 | 2.519 | 0.6810 | -31.26 | 31 |
| 1,4-Dioxane | 0.329 | 0.750 | 0.000 | 0.640 | 2.892 | 0.6810 | -30.98 | 31 |
| 2-Methyltetrahydrofuran | 0.241 | 0.480 | 0.000 | 0.530 | 2.820 | 0.7632 | -31.79 | 32 |
| 2,5-Dimethyltetrahydrofuran | 0.204 | 0.380 | 0.000 | 0.580 | 2.980 | 0.9041 | -33.31 | 32 |
| Methanol | 0.278 | 0.440 | 0.430 | 0.470 | 0.970 | 0.3082 | -16.90 | 26 |
| Ethanol | 0.246 | 0.420 | 0.370 | 0.480 | 1.485 | 0.4491 | -17.50 | 33 |
| 1-Propanol | 0.236 | 0.420 | 0.370 | 0.480 | 2.031 | 0.5900 | -22.50 | 33 |
| 1-Butanol | 0.224 | 0.420 | 0.370 | 0.480 | 2.601 | 0.7309 | -27.70 | 33 |
| 2-Propanol | 0.212 | 0.360 | 0.330 | 0.560 | 1.764 | 0.5900 | -20.80 | 33 |
| 1-Pentanol | 0.219 | 0.420 | 0.370 | 0.480 | 3.106 | 0.8718 | -31.80 | 33 |
| 1-Hexanol | 0.210 | 0.420 | 0.370 | 0.480 | 3.610 | 1.0170 | -36.40 | 34 |
| 1-Octanol | 0.199 | 0.420 | 0.370 | 0.480 | 4.619 | 1.2950 | -46.40 | 34 |
| 2-Methyl-2-butanol | 0.194 | 0.300 | 0.310 | 0.600 | 2.630 | 0.8718 | -25.44 | 16 |
| 2-Methoxyethanol | 0.269 | 0.500 | 0.300 | 0.840 | 2.490 | 0.6487 | -32.56 | 36 |
| 2-Ethoxyethanol | 0.237 | 0.520 | 0.310 | 0.810 | 2.792 | 0.7896 | -35.88 | 51 |
| Methyl acetate | 0.142 | 0.640 | 0.000 | 0.450 | 1.911 | 0.6057 | -23.94 | 37 |
| Ethyl acetate | 0.106 | 0.620 | 0.000 | 0.450 | 2.314 | 0.7466 | -27.86 | 13 |
| Propyl acetate | 0.092 | 0.600 | 0.000 | 0.450 | 2.819 | 0.8875 | -32.20 | 37 |
| Acetonitrile | 0.237 | 0.900 | 0.070 | 0.320 | 1.739 | 0.4042 | -17.93 | 13 |
| Propionitrile | 0.162 | 0.900 | 0.020 | 0.360 | 2.082 | 0.5451 | -23.50 | 38 |
| Butyronitrile | 0.180 | 0.900 | 0.000 | 0.360 | 2.548 | 0.6860 | -29.00 | 38 |
| Benzene | 0.610 | 0.520 | 0.000 | 0.140 | 2.786 | 0.7176 | -30.66 | 13 |
| Toluene | 0.601 | 0.520 | 0.000 | 0.140 | 3.325 | 0.8573 | -35.05 | 13 |
| Ethylbenzene | 0.613 | 0.510 | 0.000 | 0.150 | 3.778 | 0.9982 | -39.40 | 13 |
| 1,4-Dimethylbenzene | 0.613 | 0.520 | 0.000 | 0.160 | 3.839 | 0.9982 | -38.79 | 47 |
| Mesitylene | 0.649 | 0.520 | 0.000 | 0.190 | 4.344 | 1.1391 | -43.35 | 13 |
| Naphthalene | 1.340 | 0.920 | 0.000 | 0.200 | 5.161 | 1.0854 | -49.89 | 13 |
| Biphenyl | 1.360 | 0.990 | 0.000 | 0.260 | 6.014 | 1.3240 | -57.80 | 13 |
| Anthracene | 2.290 | 1.340 | 0.000 | 0.280 | 7.568 | 1.4540 | -72.00 | 13 |
| Acetophenone | 0.818 | 1.010 | 0.000 | 0.480 | 4.501 | 1.0140 | -42.66 | 13 |
| Anisole | 0.710 | 0.750 | 0.000 | 0.290 | 3.890 | 0.9160 | -39.62 | 13 |
| Benzaldehyde | 0.820 | 1.000 | 0.000 | 0.390 | 4.008 | 0.8730 | -39.92 | 13 |
| Benzonitrile | 0.742 | 1.110 | 0.000 | 0.330 | 4.039 | 0.8710 | -40.77 | 13 |
| Bromobenzene | 0.882 | 0.730 | 0.000 | 0.090 | 4.041 | 0.8914 | -39.33 | 13 |
| Chlorobenzene | 0.718 | 0.650 | 0.000 | 0.070 | 3.657 | 0.8388 | -37.19 | 13 |
| 1,2-Dichlorobenzene | 0.872 | 0.780 | 0.000 | 0.040 | 4.518 | 0.9612 | -42.48 | 13 |
| 1,4-Dichlorobenzene | 0.825 | 0.750 | 0.000 | 0.020 | 4.435 | 0.9612 | -42.70 | 13 |
| Hexachlorobenzene | 1.490 | 0.990 | 0.000 | 0.000 | 7.624 | 1.4508 | -64.80 | 13 |
| Fluorobenzene | 0.477 | 0.570 | 0.000 | 0.100 | 2.788 | 0.7341 | -30.92 | 13 |
| Iodobenzene | 1.188 | 0.820 | 0.000 | 0.120 | 4.502 | 0.9746 | -44.12 | 13 |
| Nitrobenzene | 0.871 | 1.110 | 0.000 | 0.280 | 4.557 | 0.8906 | -43.10 | 13 |
| Trifluoromethylbenzene | 0.225 | 0.480 | 0.000 | 0.100 | 2.894 | 0.9104 | -30.62 | 13 |

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|---|---|---|---|---|---|---|---|---|
| N-Methylpyrrole | 0.559 | 0.790 | 0.000 | 0.310 | 2.923 | 0.7180 | -32.68 | 13 |
| Aniline | 0.955 | 0.960 | 0.260 | 0.410 | 3.934 | 0.8162 | -38.12 | 24 |
| N-Methylaniline | 0.948 | 0.900 | 0.170 | 0.430 | 4.478 | 0.9571 | -43.61 | 47 |
| N-Ethylaniline | 0.945 | 0.850 | 0.170 | 0.430 | 4.811 | 1.0980 | -48.43 | 47 |
| N,N-Dimethylaniline | 0.957 | 0.810 | 0.000 | 0.410 | 4.701 | 1.0980 | -46.39 | 13 |
| Methyl methacrylate | 0.245 | 0.510 | 0.000 | 0.440 | 2.880 | 0.8445 | -30.53 | 49 |
| 3-Methylphenol | 0.822 | 0.880 | 0.570 | 0.340 | 4.310 | 0.9160 | -36.53 | 16 |
| Nitromethane | 0.313 | 0.950 | 0.060 | 0.310 | 1.892 | 0.4237 | -25.60 | 26 |
| Nitroethane | 0.270 | 0.950 | 0.020 | 0.330 | 2.414 | 0.5646 | -28.40 | 26 |
| 1-Nitropropane | 0.242 | 0.950 | 0.000 | 0.310 | 2.894 | 0.7055 | -33.00 | 26 |
| 2-Nitropropane | 0.216 | 0.920 | 0.000 | 0.330 | 2.550 | 0.7055 | -30.23 | 39 |
| Helium | 0.000 | 0.000 | 0.000 | 0.000 | -1.741 | 0.0680 | 10.13 | 35 |
| Neon | 0.000 | 0.000 | 0.000 | 0.000 | -1.575 | 0.0850 | 6.11 | 35 |
| Argon | 0.000 | 0.000 | 0.000 | 0.000 | -0.688 | 0.1900 | -0.92 | 35 |
| Krypton | 0.000 | 0.000 | 0.000 | 0.000 | -0.211 | 0.2460 | -3.56 | 35 |
| Xenon | 0.000 | 0.000 | 0.000 | 0.000 | 0.378 | 0.3290 | -10.00 | 35 |
| Hydrogen | 0.000 | 0.000 | 0.000 | 0.000 | -1.200 | 0.1086 | 5.19 | 35 |
| Nitrogen | 0.000 | 0.000 | 0.000 | 0.000 | -0.978 | 0.2222 | 2.13 | 35 |
| Carbon monoxide | 0.000 | 0.000 | 0.000 | 0.040 | -0.836 | 0.2220 | 0.84 | 35 |
| Carbon dioxide | 0.000 | 0.280 | 0.050 | 0.100 | 0.058 | 0.2809 | -6.66 | 23 |
| Oxygen | 0.000 | 0.000 | 0.000 | 0.000 | -0.723 | 0.1830 | 0.25 | 35 |
| Carbon tetrafluoride | -0.580 | -0.260 | 0.000 | 0.000 | -0.817 | 0.3203 | 0.50 | 35 |
| Sulfur hexafluoride | -0.600 | -0.200 | 0.000 | 0.000 | -0.120 | 0.4643 | -5.77 | 35 |
| Nitric oxide | 0.370 | 0.020 | 0.000 | 0.090 | -0.590 | 0.2026 | -4.46 | 40 |
| Pyridine | 0.631 | 0.840 | 0.000 | 0.520 | 3.022 | 0.6753 | -32.01 | 24 |
| 2-Methylpyridine | 0.598 | 0.750 | 0.000 | 0.580 | 3.422 | 0.8162 | -35.92 | 41 |
| 2,4-Dimethylpyridine | 0.634 | 0.760 | 0.000 | 0.630 | 4.006 | 0.9571 | -39.87 | 41 |
| 2,6-Dimethylpyridine | 0.607 | 0.700 | 0.000 | 0.630 | 3.760 | 0.9571 | -39.89 | 41 |
| 2-Chloropyridine | 0.738 | 1.030 | 0.000 | 0.370 | 3.875 | 0.7977 | -39.70 | 41 |
| 3-Chloropyridine | 0.732 | 0.830 | 0.000 | 0.400 | 3.783 | 0.7977 | -41.70 | 41 |
| 3-Cyanopyridine | 0.750 | 1.260 | 0.000 | 0.620 | 4.164 | 0.8300 | -40.50 | 41 |
| 4-Cyanopyridine | 0.750 | 1.210 | 0.000 | 0.590 | 4.033 | 0.8300 | -38.80 | 41 |
| 1-Butanethiol | 0.382 | 0.350 | 0.000 | 0.240 | 3.243 | 0.8357 | -33.32 | 42 |
| N,N-Dimethylformamide | 0.367 | 1.310 | 0.000 | 0.740 | 3.173 | 0.6468 | -34.10 | 13 |
| Dimethyl Sulfoxide | 0.522 | 1.740 | 0.000 | 0.880 | 3.459 | 0.6126 | -35.40 | 13 |
| n-Butylamine | 0.224 | 0.350 | 0.160 | 0.610 | 2.618 | 0.7720 | -29.51 | 43 |
| n-Pentylamine | 0.211 | 0.350 | 0.160 | 0.610 | 3.139 | 0.9129 | -33.95 | 43 |
| n-Hexylamine | 0.197 | 0.350 | 0.160 | 0.610 | 3.655 | 1.0538 | -39.57 | 43 |
| Octylamine | 0.187 | 0.350 | 0.160 | 0.610 | 4.520 | 1.3350 | -49.24 | 43 |
| Nonylamine | 0.187 | 0.350 | 0.160 | 0.610 | 5.100 | 1.4765 | -53.39 | 43 |
| Decylamine | 0.182 | 0.350 | 0.160 | 0.610 | 5.606 | 1.6174 | -58.15 | 43 |
| Triethylamine | 0.101 | 0.150 | 0.000 | 0.790 | 3.040 | 1.0538 | -33.80 | 46 |
| Tri-n-butylamine | 0.051 | 0.150 | 0.000 | 0.790 | 6.050 | 1.8998 | -67.51 | 13 |
| Ethyl benzoate | 0.689 | 0.850 | 0.000 | 0.460 | 5.075 | 1.2140 | -52.55 | 45 |
| Dimethoxymethane | 0.099 | 0.460 | 0.000 | 0.520 | 1.894 | 0.6487 | -23.74 | 44 |
| Propyl propionate | 0.070 | 0.560 | 0.000 | 0.450 | 3.338 | 1.0284 | -38.21 | 117 |
| Propionaldehyde | 0.196 | 0.650 | 0.000 | 0.450 | 1.815 | 0.5470 | -21.38 | 14 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Carbon disulfide | 0.876 | 0.260 | 0.000 | 0.030 | 2.370 | 0.4905 | -26.11 | 14 |
| Methyl propanoate | 0.128 | 0.600 | 0.000 | 0.450 | 2.431 | 0.7466 | -27.61 | 14 |
| 1,2-Dimethoxyethane | 0.116 | 0.670 | 0.000 | 0.680 | 2.654 | 0.7896 | -29.50 | 14 |
| Hexafluorobenzene | 0.088 | 0.560 | 0.000 | 0.010 | 2.345 | 0.8226 | -27.15 | 14 |
| Trichloroethene | 0.524 | 0.370 | 0.080 | 0.030 | 2.997 | 0.7146 | -32.21 | 14 |
| 1,4-Difluorobenzene | 0.384 | 0.600 | 0.000 | 0.060 | 2.766 | 0.7518 | -30.92 | 14 |
| 1-Iodopropane | 0.634 | 0.400 | 0.000 | 0.150 | 3.130 | 0.7895 | -32.97 | 14 |
| Butyl acetate | 0.071 | 0.600 | 0.000 | 0.450 | 3.353 | 1.0284 | -37.40 | 14 |
| 1-Decanol | 0.191 | 0.420 | 0.370 | 0.480 | 5.628 | 1.5763 | -56.27 | 14 |
| Phenanthrene | 2.055 | 1.290 | 0.000 | 0.260 | 7.632 | 1.4540 | -68.70 | 14 |
| Benzil | 1.445 | 1.590 | 0.000 | 0.620 | 7.611 | 1.6374 | -65.98 | 14 |
| Adamantane | 0.760 | 0.570 | 0.000 | 0.040 | 4.934 | 1.1918 | -49.30 | 109 |
| Iodomethane | 0.676 | 0.430 | 0.000 | 0.120 | 2.106 | 0.5077 | -24.27 | 120 |
| 1-Iodobutane | 0.628 | 0.400 | 0.000 | 0.150 | 3.628 | 0.9304 | -35.55 | 120 |
| 2-Chloro-2-methylpropane | 0.142 | 0.300 | 0.000 | 0.030 | 2.273 | 0.7946 | -26.74 | 120 |
| 2-Iodo-2-methylpropane | 0.589 | 0.350 | 0.000 | 0.190 | 3.439 | 0.9304 | -33.39 | 120 |
| Sulfur dioxide | 0.370 | 0.660 | 0.280 | 0.100 | 0.778 | 0.3465 | -14.64 | 4 |
| 1-Bromoadamantane | 1.070 | 0.900 | 0.000 | 0.200 | 6.130 | 1.3668 | -58.40 | 11 |
| 1-Adamantanol | 0.940 | 0.900 | 0.310 | 0.660 | 5.634 | 1.2505 | -57.60 | 11 |

TABLE S4. Values of the gas to benzene solvation enthalpy in kJ/mol at 298K for 174 solutes, together with the solute descriptors.

| Solute | **E** | **S** | **A** | **B** | **L** | **V** | Exp Value | Ref. |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Methane | 0.000 | 0.000 | 0.000 | 0.000 | -0.323 | 0.2495 | -1.26 | 35 |
| Ethane | 0.000 | 0.000 | 0.000 | 0.000 | 0.492 | 0.3904 | -8.37 | 35 |
| Propane | 0.000 | 0.000 | 0.000 | 0.000 | 1.050 | 0.5313 | -13.39 | 35 |
| 2-Methylpropane | 0.000 | 0.000 | 0.000 | 0.000 | 1.409 | 0.6722 | -15.48 | 35 |
| Butane | 0.000 | 0.000 | 0.000 | 0.000 | 1.615 | 0.6722 | -17.41 | 35 |
| Pentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.162 | 0.8131 | -22.13 | 18 |
| Hexane | 0.000 | 0.000 | 0.000 | 0.000 | 2.668 | 0.9540 | -26.65 | 18 |
| Heptane | 0.000 | 0.000 | 0.000 | 0.000 | 3.173 | 1.0949 | -31.00 | 18 |
| Octane | 0.000 | 0.000 | 0.000 | 0.000 | 3.677 | 1.2358 | -35.48 | 18 |
| Nonane | 0.000 | 0.000 | 0.000 | 0.000 | 4.182 | 1.3767 | -39.66 | 18 |
| Decane | 0.000 | 0.000 | 0.000 | 0.000 | 4.686 | 1.5176 | -43.85 | 18 |
| Dodecane | 0.000 | 0.000 | 0.000 | 0.000 | 5.696 | 1.7994 | -52.30 | 18 |
| Tetradecane | 0.000 | 0.000 | 0.000 | 0.000 | 6.705 | 2.0812 | -61.63 | 84 |
| Hexadecane | 0.000 | 0.000 | 0.000 | 0.000 | 7.714 | 2.3630 | -70.08 | 18 |
| 2-Methylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.013 | 0.6722 | -20.50 | 118 |
| 3-Ethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.091 | 1.0949 | -30.00 | 15 |
| 2,2-Dimethylbutane | 0.000 | 0.000 | 0.000 | 0.000 | 2.352 | 0.9540 | -22.88 | 24 |
| 2,2-Dimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 2.796 | 1.0949 | -26.94 | 24 |
| 3,3-Diethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.820 | 1.0949 | -36.86 | 24 |
| 2-Methyloctane | 0.000 | 0.000 | 0.000 | 0.000 | 3.966 | 1.3767 | -38.03 | 24 |
| 2,2,4-Trimethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.106 | 1.2358 | -29.16 | 24 |
| 2,2,4,4-Tetramethylpentane | 0.000 | 0.000 | 0.000 | 0.000 | 3.512 | 1.3767 | -32.01 | 24 |
| 2,2,5,5-Tetramethylhexane | 0.000 | 0.000 | 0.000 | 0.000 | 4.039 | 1.5176 | -34.43 | 24 |
| Cyclopentane | 0.263 | 0.100 | 0.000 | 0.000 | 2.477 | 0.7045 | -25.65 | 24 |
| Cyclohexane | 0.305 | 0.100 | 0.000 | 0.000 | 2.964 | 0.8454 | -29.41 | 24 |
| Cycloheptane | 0.350 | 0.100 | 0.000 | 0.000 | 3.704 | 0.9863 | -35.34 | 85 |
| Cyclooctane | 0.413 | 0.100 | 0.000 | 0.000 | 4.329 | 1.1272 | -39.68 | 85 |
| Methylcyclohexane | 0.244 | 0.060 | 0.000 | 0.000 | 3.319 | 0.9863 | -31.30 | 24 |
| *cis*-1,2-Dimethylcyclohexane | 0.281 | 0.240 | 0.000 | 0.000 | 3.847 | 1.1272 | -35.27 | 24 |
| *cis* Decalin | 0.550 | 0.250 | 0.000 | 0.000 | 5.156 | 1.3004 | -46.43 | 124 |
| Ethene | 0.107 | 0.100 | 0.000 | 0.070 | 0.289 | 0.3474 | -9.00 | 27 |
| 1-Butene | 0.100 | 0.080 | 0.000 | 0.070 | 1.491 | 0.6292 | -18.53 | 121 |
| *cis* 2-Butene | 0.140 | 0.080 | 0.000 | 0.050 | 1.737 | 0.6292 | -20.95 | 121 |
| *trans* 2-Butene | 0.126 | 0.080 | 0.000 | 0.050 | 1.664 | 0.6292 | -19.23 | 121 |
| 2-Methylpropene | 0.120 | 0.080 | 0.000 | 0.080 | 1.579 | 0.6292 | -19.10 | 121 |
| 1-Pentene | 0.093 | 0.080 | 0.000 | 0.070 | 2.047 | 0.7701 | -22.92 | 24 |
| 1-Hexene | 0.078 | 0.080 | 0.000 | 0.070 | 2.572 | 0.9110 | -27.91 | 24 |
| 1-Heptene | 0.092 | 0.080 | 0.000 | 0.070 | 3.063 | 1.0519 | -32.47 | 24 |
| 1-Octene | 0.094 | 0.080 | 0.000 | 0.070 | 3.568 | 1.1928 | -36.69 | 24 |
| 1-Nonene | 0.090 | 0.080 | 0.000 | 0.070 | 4.073 | 1.3337 | -41.21 | 24 |
| 1-Decene | 0.090 | 0.080 | 0.000 | 0.070 | 4.554 | 1.4746 | -45.56 | 24 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1-Dodecene | 0.089 | 0.080 | 0.000 | 0.070 | 5.515 | 1.7564 | -54.52 | 24 |
| 1-Tridecene | 0.087 | 0.080 | 0.000 | 0.070 | 6.020 | 1.8973 | -59.07 | 24 |
| 1-Tetradecene | 0.085 | 0.080 | 0.000 | 0.070 | 6.513 | 2.0382 | -63.43 | 24 |
| 1-Pentadecene | 0.083 | 0.080 | 0.000 | 0.070 | 7.006 | 2.1791 | -67.82 | 24 |
| *cis* 2-Octene | 0.135 | 0.080 | 0.000 | 0.070 | 3.683 | 1.1928 | -35.98 | 24 |
| *trans* 2-Octene | 0.123 | 0.080 | 0.000 | 0.070 | 3.600 | 1.1928 | -35.81 | 24 |
| *cis* 4-Octene | 0.133 | 0.080 | 0.000 | 0.070 | 3.607 | 1.1928 | -35.44 | 24 |
| *trans* 4-Octene | 0.144 | 0.080 | 0.000 | 0.070 | 3.593 | 1.1928 | -35.31 | 24 |
| 1,3-Butadiene | 0.320 | 0.230 | 0.000 | 0.100 | 1.543 | 0.5862 | -20.28 | 121 |
| 1,5-Hexadiene | 0.191 | 0.150 | 0.000 | 0.100 | 2.450 | 0.8680 | -29.20 | 24 |
| Cyclopentene | 0.335 | 0.200 | 0.000 | 0.100 | 2.402 | 0.6605 | -26.27 | 24 |
| Cyclohexene | 0.395 | 0.200 | 0.000 | 0.100 | 3.021 | 0.8025 | -31.51 | 24 |
| 1-Methylcyclohexene | 0.391 | 0.200 | 0.000 | 0.100 | 3.483 | 0.9433 | -34.94 | 24 |
| Norbornadiene | 0.495 | 0.320 | 0.000 | 0.110 | 3.108 | 0.7919 | -33.66 | 25 |
| Acetone | 0.179 | 0.700 | 0.040 | 0.490 | 1.696 | 0.5470 | -30.08 | 19 |
| 2-Butanone | 0.166 | 0.700 | 0.000 | 0.510 | 2.287 | 0.6879 | -34.27 | 19 |
| 2-Pentanone | 0.143 | 0.680 | 0.000 | 0.510 | 2.755 | 0.8288 | -37.61 | 29 |
| 3-Pentanone | 0.154 | 0.660 | 0.000 | 0.510 | 2.811 | 0.8288 | -38.58 | 29 |
| 2-Hexanone | 0.136 | 0.680 | 0.000 | 0.510 | 3.286 | 0.9697 | -42.17 | 29 |
| 3-Hexanone | 0.136 | 0.660 | 0.000 | 0.510 | 3.310 | 0.9697 | -41.97 | 29 |
| 2-Heptanone | 0.123 | 0.680 | 0.000 | 0.510 | 3.760 | 1.1106 | -46.44 | 19 |
| 4-Heptanone | 0.110 | 0.660 | 0.000 | 0.510 | 3.705 | 1.1106 | -45.81 | 19 |
| 2-Octanone | 0.108 | 0.680 | 0.000 | 0.510 | 4.257 | 1.2515 | -50.84 | 29 |
| 2-Nonanone | 0.119 | 0.680 | 0.000 | 0.510 | 4.735 | 1.3924 | -54.98 | 19 |
| 5-Nonanone | 0.103 | 0.660 | 0.000 | 0.510 | 4.698 | 1.3924 | -53.35 | 19 |
| 2-Decanone | 0.108 | 0.680 | 0.000 | 0.510 | 5.245 | 1.5333 | -58.62 | 29 |
| 2-Undecanone | 0.101 | 0.680 | 0.000 | 0.510 | 5.732 | 1.6740 | -62.80 | 29 |
| 6-Undecanone | 0.083 | 0.660 | 0.000 | 0.510 | 5.677 | 1.6740 | -61.37 | 29 |
| 3,3-Dimethyl-2-butanone | 0.106 | 0.620 | 0.000 | 0.510 | 2.928 | 0.9697 | -37.66 | 29 |
| 2,2,4,4-Tetramethyl-3-pentanone | 0.099 | 0.560 | 0.000 | 0.520 | 4.370 | 1.3924 | -43.01 | 19 |
| Cyclopentanone | 0.373 | 0.860 | 0.000 | 0.520 | 3.221 | 0.7200 | -43.72 | 29 |
| Cyclohexanone | 0.403 | 0.860 | 0.000 | 0.560 | 3.792 | 0.8610 | -46.16 | 19 |
| Cycloheptanone | 0.436 | 0.860 | 0.000 | 0.560 | 4.376 | 1.0020 | -49.62 | 29 |
| Dimethyl ether | 0.000 | 0.270 | 0.000 | 0.410 | 1.285 | 0.4491 | -21.10 | 121 |
| Diethyl ether | 0.041 | 0.250 | 0.000 | 0.450 | 2.015 | 0.7309 | -26.36 | 118 |
| Dibutyl ether | 0.000 | 0.250 | 0.000 | 0.450 | 3.924 | 1.2950 | -42.17 | 114 |
| Methyl butyl ether | 0.045 | 0.250 | 0.000 | 0.440 | 2.658 | 0.8718 | -31.38 | 118 |
| Methyl heptyl ether | 0.048 | 0.250 | 0.000 | 0.450 | 4.088 | 1.2950 | -44.81 | 114 |
| Methyl *tert*-butyl ether | 0.024 | 0.210 | 0.000 | 0.590 | 2.380 | 0.8718 | -28.03 | 118 |
| Methyl *tert*-amyl ether | 0.050 | 0.210 | 0.000 | 0.600 | 2.916 | 1.0170 | -34.61 | 88 |
| Tetrahydrofuran | 0.289 | 0.520 | 0.000 | 0.480 | 2.636 | 0.6223 | -31.80 | 94 |
| 1,3-Dioxane | 0.308 | 0.720 | 0.000 | 0.700 | 2.519 | 0.6810 | -39.77 | 31 |
| 1,4-Dioxane | 0.329 | 0.750 | 0.000 | 0.640 | 2.892 | 0.6810 | -39.03 | 31 |
| 2-Methyltetrahydrofuran | 0.241 | 0.480 | 0.000 | 0.530 | 2.820 | 0.7632 | -34.16 | 87 |
| Diglyme | 0.113 | 0.760 | 0.000 | 1.170 | 3.920 | 1.1301 | -49.00 | 129 |
| 15-Crown-5 | 0.410 | 1.200 | 0.000 | 1.750 | 6.779 | 1.7025 | -81.45 | 88 |
| 18-Crown-6 | 0.400 | 1.340 | 0.000 | 2.130 | 7.919 | 2.0430 | -100.80 | 89 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1-Butanol | 0.224 | 0.420 | 0.370 | 0.480 | 2.601 | 0.7309 | -35.14 | 118 |
| 1-Pentanol | 0.219 | 0.420 | 0.370 | 0.480 | 3.106 | 0.8718 | -39.33 | 118 |
| 1-Hexanol | 0.210 | 0.420 | 0.370 | 0.480 | 3.610 | 1.0170 | -49.66 | 90 |
| 1-Octanol | 0.199 | 0.420 | 0.370 | 0.480 | 4.619 | 1.2950 | -52.76 | 114 |
| 1-Decanol | 0.191 | 0.420 | 0.370 | 0.480 | 5.628 | 1.5763 | -65.00 | 125 |
| *tert*-Butanol | 0.180 | 0.300 | 0.310 | 0.600 | 1.963 | 0.7309 | -34.00 | 91 |
| 2-Methyl-2-butanol | 0.194 | 0.300 | 0.310 | 0.600 | 2.630 | 0.8718 | -33.47 | 118 |
| 2-Ethoxyethanol | 0.237 | 0.520 | 0.310 | 0.810 | 2.792 | 0.7896 | -39.43 | 92 |
| 1,1-Difluoroethane | -0.250 | 0.470 | 0.040 | 0.070 | 0.570 | 0.4258 | -18.13 | 121 |
| 1-Fluorooctane | -0.020 | 0.350 | 0.000 | 0.100 | 3.850 | 1.2538 | -47.61 | 114 |
| Chloroethane | 0.227 | 0.400 | 0.000 | 0.100 | 1.678 | 0.5128 | -25.62 | 121 |
| 1-Chlorohexane | 0.201 | 0.400 | 0.000 | 0.100 | 3.777 | 1.0770 | -41.97 | 127 |
| 1-Chlorooctane | 0.191 | 0.400 | 0.000 | 0.090 | 4.708 | 1.3585 | -50.38 | 114 |
| 1,1,2,2-Tetrachloroethane | 0.595 | 0.760 | 0.160 | 0.120 | 3.803 | 0.8800 | -47.72 | 122 |
| Phenol | 0.805 | 0.890 | 0.600 | 0.300 | 3.766 | 0.7751 | -49.95 | 93 |
| 2,6-Dimethylphenol | 0.850 | 0.820 | 0.510 | 0.370 | 4.495 | 1.0569 | -52.59 | 94 |
| 1-Naphthol | 1.520 | 1.050 | 0.600 | 0.370 | 6.130 | 1.1441 | -69.20 | 128 |
| Dimethyl sulfoxide | 0.522 | 1.720 | 0.000 | 0.970 | 3.459 | 0.6126 | -48.08 | 93 |
| Pyridine | 0.631 | 0.840 | 0.000 | 0.520 | 3.022 | 0.6753 | -40.20 | 93 |
| 2-Methylpyridine | 0.598 | 0.750 | 0.000 | 0.580 | 3.422 | 0.8162 | -42.43 | 41 |
| 2,4-Dimethylpyridine | 0.634 | 0.760 | 0.000 | 0.630 | 4.006 | 0.9571 | -47.04 | 41 |
| 2,6-Dimethylpyridine | 0.607 | 0.700 | 0.000 | 0.630 | 3.760 | 0.9571 | -45.00 | 41 |
| 2-Chloropyridine | 0.738 | 1.030 | 0.000 | 0.370 | 3.875 | 0.7977 | -47.90 | 41 |
| 3-Chloropyridine | 0.732 | 0.830 | 0.000 | 0.400 | 3.783 | 0.7977 | -48.50 | 41 |
| 3-Cyanopyridine | 0.750 | 1.260 | 0.000 | 0.620 | 4.164 | 0.8300 | -54.10 | 41 |
| 4-Cyanopyridine | 0.750 | 1.210 | 0.000 | 0.590 | 4.033 | 0.8300 | -55.00 | 41 |
| Triethylamine | 0.101 | 0.150 | 0.000 | 0.790 | 3.040 | 1.0538 | -37.06 | 93 |
| Nitric oxide | 0.370 | 0.020 | 0.000 | 0.090 | -0.590 | 0.2026 | 2.45 | 40 |
| Helium | 0.000 | 0.000 | 0.000 | 0.000 | -1.741 | 0.0680 | 10.29 | 35 |
| Neon | 0.000 | 0.000 | 0.000 | 0.000 | -1.575 | 0.0850 | 10.46 | 35 |
| Argon | 0.000 | 0.000 | 0.000 | 0.000 | -0.688 | 0.1900 | 1.26 | 35 |
| Krypton | 0.000 | 0.000 | 0.000 | 0.000 | -0.211 | 0.2460 | -1.92 | 35 |
| Xenon | 0.000 | 0.000 | 0.000 | 0.000 | 0.378 | 0.3290 | -7.11 | 35 |
| Radon | 0.000 | 0.000 | 0.000 | 0.000 | 0.877 | 0.3840 | -13.31 | 35 |
| Hydrogen | 0.000 | 0.000 | 0.000 | 0.000 | -1.200 | 0.1086 | 6.36 | 35 |
| Nitrogen | 0.000 | 0.000 | 0.000 | 0.000 | -0.978 | 0.2222 | 4.27 | 35 |
| Carbon Monoxide | 0.000 | 0.000 | 0.000 | 0.040 | -0.836 | 0.2220 | 2.68 | 35 |
| Carbon Dioxide | 0.000 | 0.280 | 0.050 | 0.100 | 0.058 | 0.2809 | -9.20 | 95 |
| Oxygen | 0.000 | 0.000 | 0.000 | 0.000 | -0.723 | 0.1830 | 1.72 | 35 |
| Tetrafluoromethane | -0.580 | -0.260 | 0.000 | 0.000 | -0.817 | 0.3202 | 2.26 | 35 |
| Sulfur hexafluoride | -0.600 | -0.200 | 0.000 | 0.000 | -0.120 | 0.4643 | -3.26 | 35 |
| Sulfur dioxide | 0.370 | 0.660 | 0.280 | 0.100 | 0.778 | 0.3465 | -24.27 | 4 |
| Benzene | 0.610 | 0.520 | 0.000 | 0.140 | 2.786 | 0.7176 | -33.85 | 118 |
| Toluene | 0.601 | 0.520 | 0.000 | 0.140 | 3.325 | 0.8573 | -37.66 | 118 |
| 1,4-Dimethylbenzene | 0.613 | 0.520 | 0.000 | 0.160 | 3.839 | 0.9982 | -42.15 | 45 |
| Mesitylene | 0.649 | 0.520 | 0.000 | 0.190 | 4.344 | 1.1391 | -44.77 | 118 |
| Naphthalene | 1.340 | 0.920 | 0.000 | 0.200 | 5.161 | 1.0854 | -55.28 | 69 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Phenanthrene | 2.055 | 1.290 | 0.000 | 0.260 | 7.632 | 1.4540 | -74.04 | 69 |
| Biphenyl | 1.360 | 0.990 | 0.000 | 0.260 | 6.014 | 1.3240 | -63.40 | 123 |
| 1,3-Dichlorobenzene | 0.847 | 0.730 | 0.000 | 0.020 | 4.410 | 0.9612 | -45.95 | 96 |
| Anisole | 0.710 | 0.750 | 0.000 | 0.290 | 3.890 | 0.9160 | -46.58 | 97 |
| γ-Butyrolactone | 0.387 | 1.380 | 0.000 | 0.590 | 3.326 | 0.6380 | -53.92 | 98 |
| Ethyl acetate | 0.106 | 0.620 | 0.000 | 0.450 | 2.314 | 0.7466 | -34.74 | 119 |
| Difluorodichloromethane | 0.037 | 0.040 | 0.000 | 0.040 | 0.998 | 0.5297 | -18.58 | 28 |
| Ethyl formate | 0.146 | 0.660 | 0.000 | 0.380 | 1.845 | 0.6057 | -30.38 | 99 |
| 1-Butanethiol | 0.382 | 0.350 | 0.000 | 0.240 | 3.243 | 0.8357 | -35.79 | 42 |
| Methyl methacrylate | 0.245 | 0.510 | 0.000 | 0.440 | 2.880 | 0.8445 | -38.44 | 49 |
| Benzonitrile | 0.742 | 1.110 | 0.000 | 0.330 | 4.039 | 0.8710 | -52.03 | 100 |
| Chlorotrifluoromethane | -0.247 | -0.046 | 0.000 | 0.000 | 0.209 | 0.4250 | -5.02 | 27 |
| Diiodomethane | 0.714 | 0.690 | 0.110 | 0.070 | 2.886 | 0.7659 | -45.02 | 110 |
| Nitrobenzene | 0.871 | 1.110 | 0.000 | 0.280 | 4.557 | 0.8906 | -52.72 | 118 |
| Trifluoromethylbenzene | 0.225 | 0.480 | 0.000 | 0.100 | 2.894 | 0.9104 | -35.15 | 118 |
| 3-Methylphenol | 0.822 | 0.880 | 0.570 | 0.340 | 4.310 | 0.9160 | -51.04 | 118 |
| Ethyl benzoate | 0.689 | 0.850 | 0.000 | 0.460 | 5.075 | 1.2140 | -58.78 | 45 |
| Acetonitrile | 0.237 | 0.900 | 0.070 | 0.320 | 1.739 | 0.4042 | -31.23 | 101 |
| 1-Nitropropane | 0.242 | 0.950 | 0.000 | 0.310 | 2.894 | 0.7055 | -43.37 | 39 |
| 2-Nitropropane | 0.216 | 0.920 | 0.000 | 0.330 | 2.550 | 0.7055 | -40.30 | 39 |
| Nitromethane | 0.313 | 0.950 | 0.060 | 0.310 | 1.892 | 0.4237 | -35.01 | 74 |
| Nitroethane | 0.270 | 0.950 | 0.020 | 0.330 | 2.414 | 0.5646 | -38.29 | 102 |
| Fluorobenzene | 0.477 | 0.570 | 0.000 | 0.100 | 2.788 | 0.7341 | -35.44 | 45 |
| Chlorobenzene | 0.718 | 0.650 | 0.000 | 0.070 | 3.657 | 0.8388 | -40.83 | 45 |
| Bromobenzene | 0.882 | 0.730 | 0.000 | 0.090 | 4.041 | 0.8914 | -43.60 | 45 |
| Iodobenzene | 1.188 | 0.820 | 0.000 | 0.120 | 4.502 | 0.9746 | -48.76 | 45 |
| Aniline | 0.955 | 0.960 | 0.260 | 0.410 | 3.934 | 0.8162 | -50.54 | 15 |
| Carbon Tetrachloride | 0.458 | 0.380 | 0.000 | 0.000 | 2.823 | 0.7391 | -31.88 | 24 |
| Chloroform | 0.425 | 0.490 | 0.150 | 0.020 | 2.480 | 0.6167 | -32.27 | 103 |
| Dimethoxymethane | 0.099 | 0.460 | 0.000 | 0.520 | 1.894 | 0.6487 | -28.12 | 44 |
| 1,2-Dimethoxyethane | 0.116 | 0.670 | 0.000 | 0.680 | 2.654 | 0.7896 | -37.21 | 104 |
| Ethanol | 0.246 | 0.420 | 0.370 | 0.480 | 1.485 | 0.4491 | -29.62 | 105 |
| Benzaldehyde | 0.820 | 1.000 | 0.000 | 0.390 | 4.008 | 0.8730 | -48.95 | 111 |
| 1-Nitronaphthalene | 1.337 | 0.940 | 0.000 | 0.220 | 5.802 | 1.2596 | -68.20 | 111 |
| 4-Chloronitrobenzene | 0.980 | 1.180 | 0.000 | 0.240 | 5.220 | 1.0130 | -55.23 | 111 |
| 1,4-Dibromobenzene | 1.150 | 0.860 | 0.000 | 0.040 | 5.324 | 1.0664 | -54.54 | 108 |
| 4-Nitrotoluene | 0.870 | 1.110 | 0.000 | 0.280 | 5.154 | 1.0135 | -61.33 | 108 |
| Pyrrole | 0.613 | 0.730 | 0.410 | 0.290 | 2.865 | 0.5570 | -42.10 | 126 |
| N-Methylpyrrole | 0.559 | 0.790 | 0.000 | 0.310 | 2.923 | 0.7180 | -40.02 | 126 |

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