

Supplementary Material

Predicting partition coefficients in organic biphasic systems using COSMO-RS

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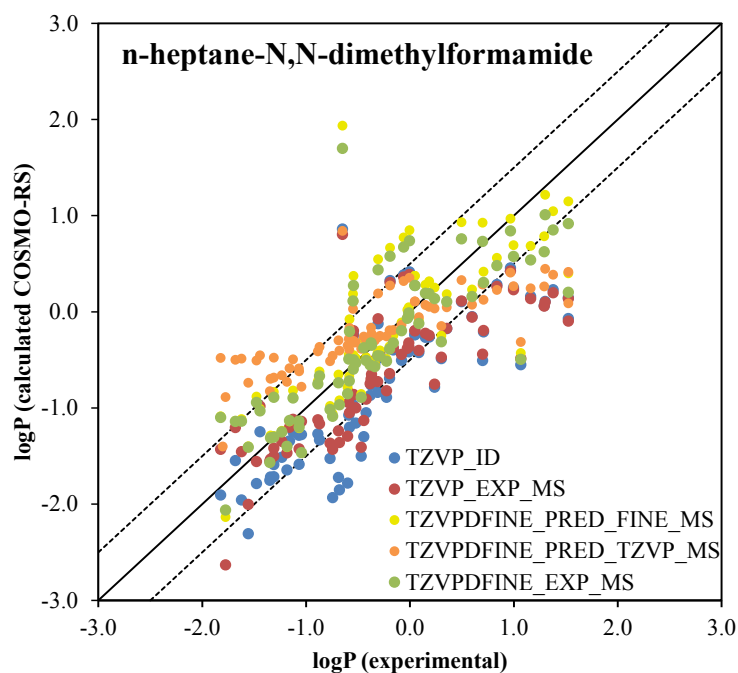
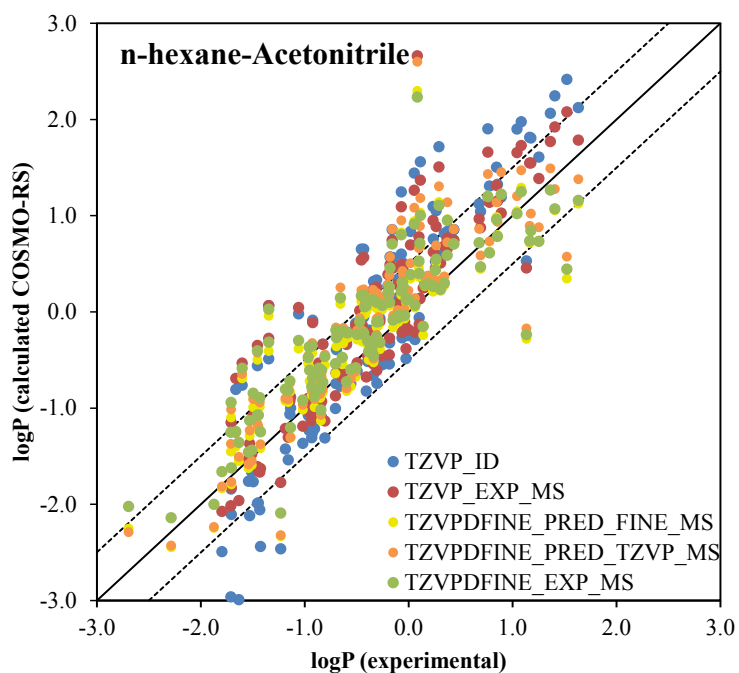


Figure S1: Calculated vs experimental partition coefficients of (A) n-hexane-acetonitrile system and (B) n-heptane-N,N-dimethylformamide at 25 °C by using different parametrizations and mutual solubilities definition.

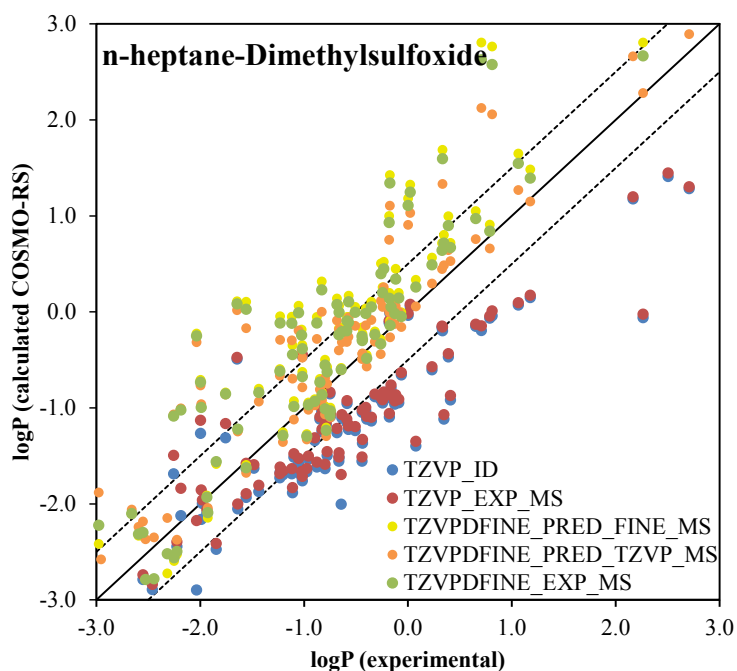
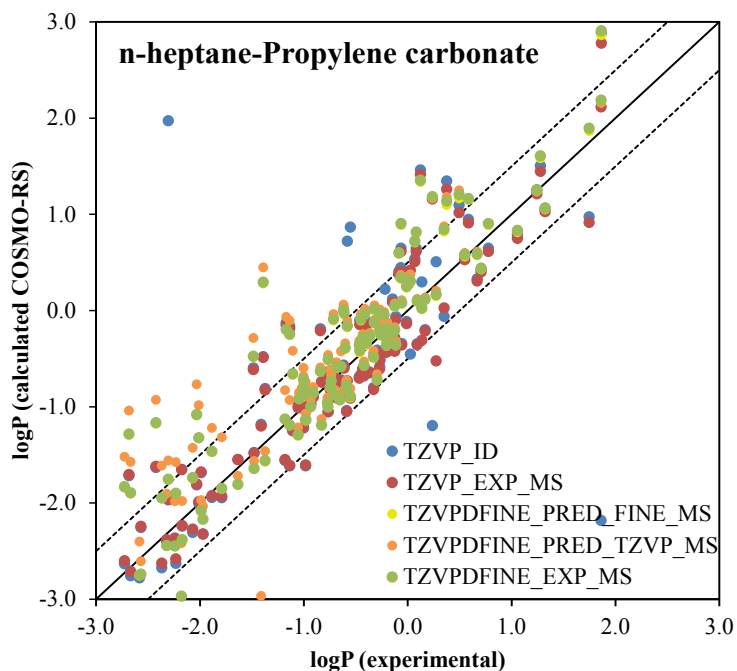


Figure S2: Calculated vs experimental partition coefficients of (A) n-heptane-propylene carbonate system and (B) n-heptane-dimethylsulfoxide at 25 °C by using different parametrizations and mutual solubilities definition

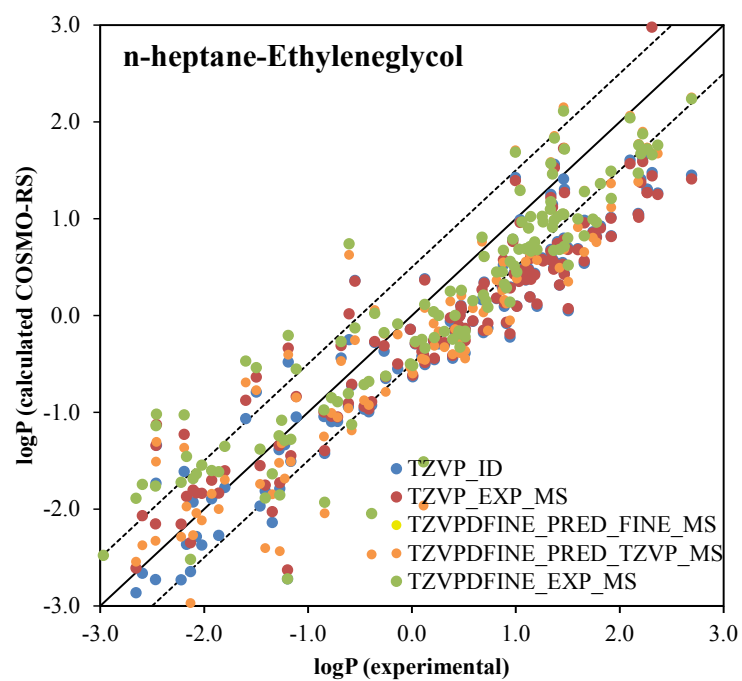


Figure S3: Calculated vs experimental partition coefficients of n-heptane-ethylene glycol at 25 °C by using different parametrizations and mutual solubilities definition

Table S1: Experimental (literature) and calculated mutual solubilities of the different binary organic biphasic systems at 25 °C.

| Solvent 1 | Solvent 2 | Experimental | | | | COSMO-RS TZVPD_FINE | | | | COSMO-RS TZVP | | | |
|-------------|-------------------------------|----------------|----------------|----------------|----------------|---------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| | | Bottom phase | | Top phase | | Bottom phase | | Top phase | | Bottom phase | | Top phase | |
| | | x ₁ | x ₂ | x ₁ | x ₂ | x ₁ | x ₂ | x ₁ | x ₂ | x ₁ | x ₂ | x ₁ | x ₂ |
| n-Hexane | Acetonitrile | 0.0567 | 0.9433 | 0.9416 | 0.0584 | 0.0477 | 0.9523 | 0.9682 | 0.0318 | 0.0130 | 0.9870 | 0.9699 | 0.0301 |
| n-Heptane | Methanol | 0.1165 | 0.8835 | 0.8319 | 0.1681 | 0.0200 | 0.9800 | 0.9500 | 0.0500 | 0.0200 | 0.9800 | 0.9900 | 0.0100 |
| n-Heptane | <i>N,N</i> -Dimethylformamide | 0.0956 | 0.9044 | 0.9759 | 0.0241 | 0.0500 | 0.9500 | 0.9800 | 0.0200 | 0.3000 | 0.7000 | 0.8000 | 0.2000 |
| n-Heptane | Dimethyl sulfoxide | 0.0130 | 0.9870 | 0.9975 | 0.0025 | 0.0010 | 0.9990 | 0.9990 | 0.0010 | 0.0500 | 0.9500 | 0.9900 | 0.0100 |
| n-Heptane | Ethylene glycol | 0.0044 | 0.9956 | 0.9899 | 0.0101 | 0.0010 | 0.9990 | 1.0000 | 0.0000 | 0.0010 | 0.9990 | 1.0000 | 0.0000 |
| n-Heptane | 3,3,3-Trifluoroethanol | 0.0140 | 0.9860 | 0.9739 | 0.0261 | 0.0200 | 0.9800 | 0.9800 | 0.0200 | 0.0100 | 0.9900 | 0.9900 | 0.0100 |
| n-Heptane | Propylene carbonate | 0.0150 | 0.9850 | 0.9990 | 0.0010 | 0.0200 | 0.9800 | 0.9990 | 0.0010 | 0.0200 | 0.9800 | 0.9900 | 0.0100 |
| n-Heptane | Formamide | 0.0007 | 0.9993 | 1.0000 | 0.0000 | 0.0005 | 0.9995 | 0.9994 | 0.0006 | 0.0000 | 1.0000 | 1.0000 | 0.0000 |
| n-Heptane | Ethanolamine | 0.0011 | 0.9989 | 0.9980 | 0.0020 | 0.0395 | 0.9605 | 0.8906 | 0.1094 | 0.0500 | 0.9500 | 0.9500 | 0.0500 |
| RMSD | | | | | | 0.04 | 0.04 | 0.05 | 0.05 | 0.08 | 0.08 | 0.08 | 0.08 |
| MAD | | | | | | 0.024 | 0.024 | 0.03 | 0.03 | 0.049 | 0.049 | 0.05 | 0.05 |

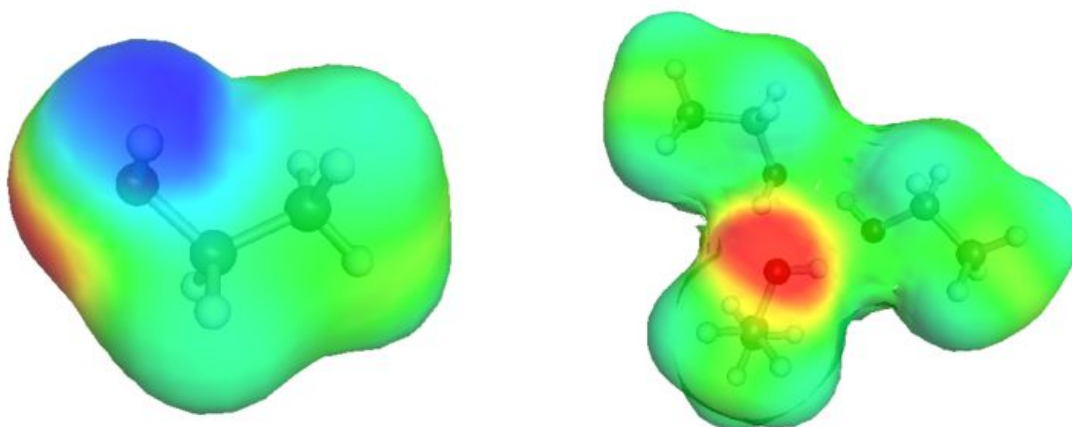


Figure S4: σ -surfaces of the ethanol monomer (A) and trimer (B) conformations

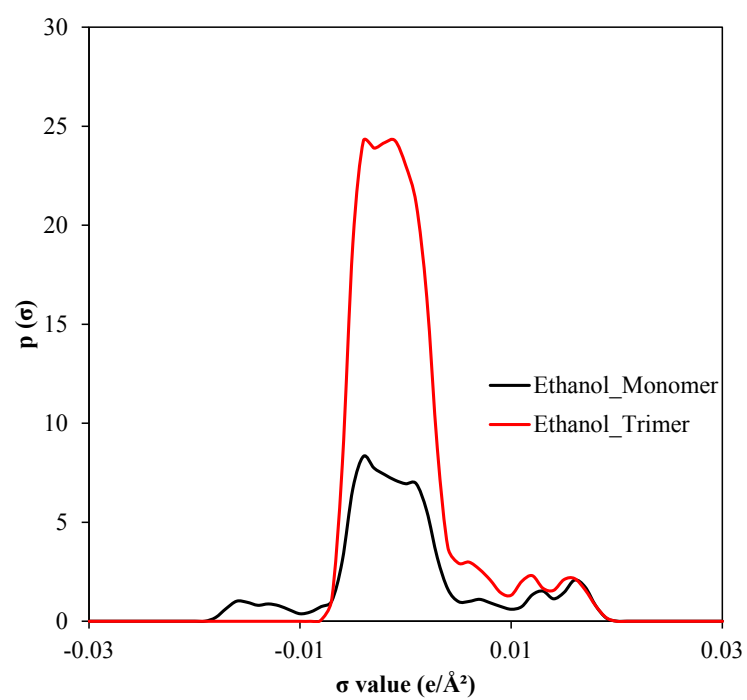


Figure S5: σ -profile of ethanol monomer and trimer conformations

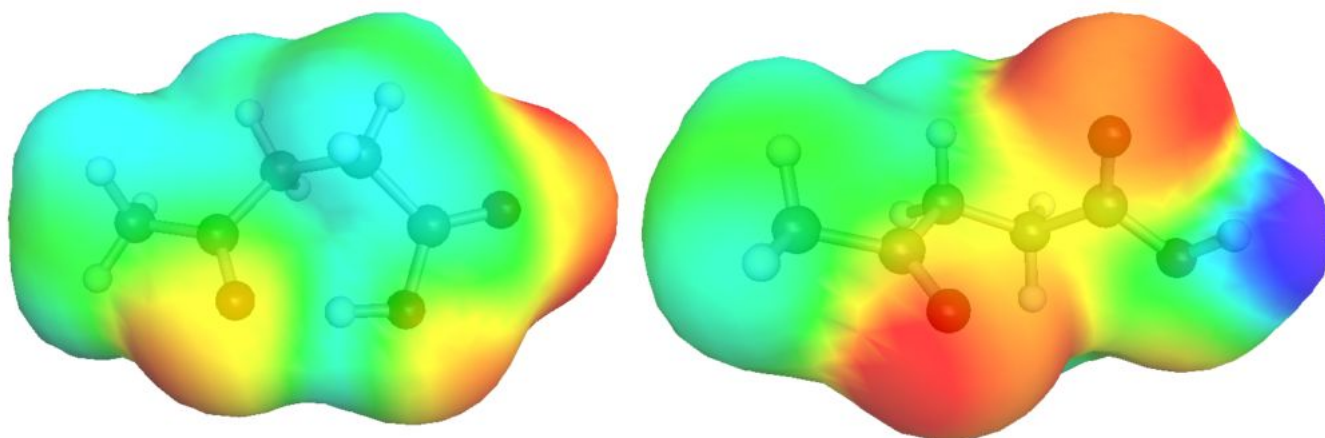


Figure S6: σ -surface of the most stable levulinic acid conformer (A) and the second one (B).

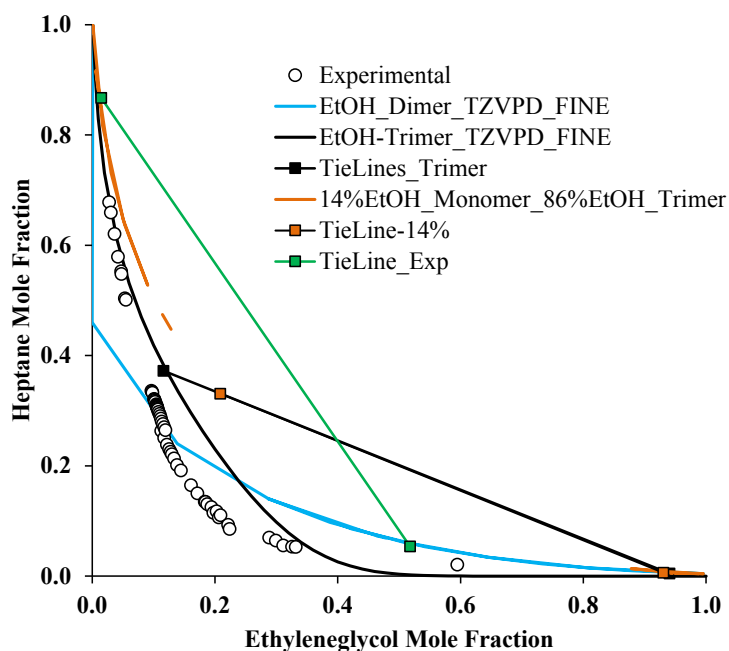
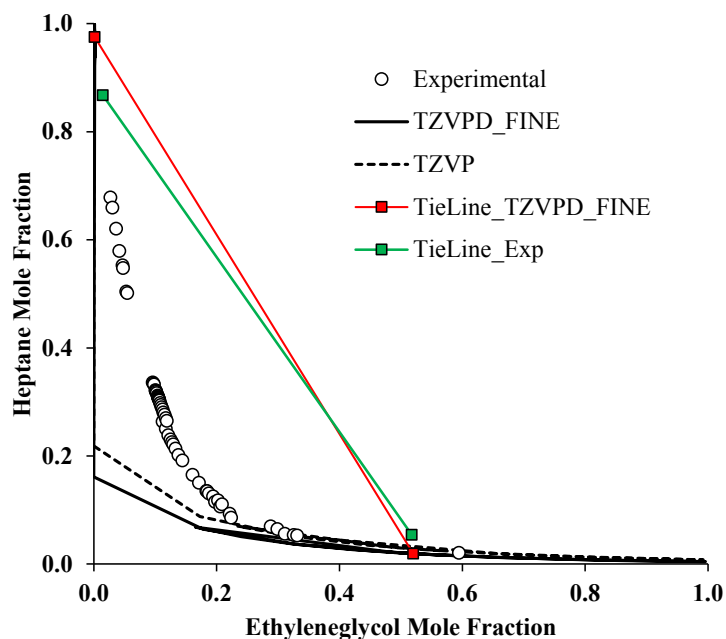


Figure S6. Experimental vs calculated binodal curves and tie lines by using ethanol monomer (A) and ethanol trimer approximation (B) with TZVP and TZVPD_FINE parametrizations at 25 °C in n-heptane/ethanol/ethylene glycol OBS.

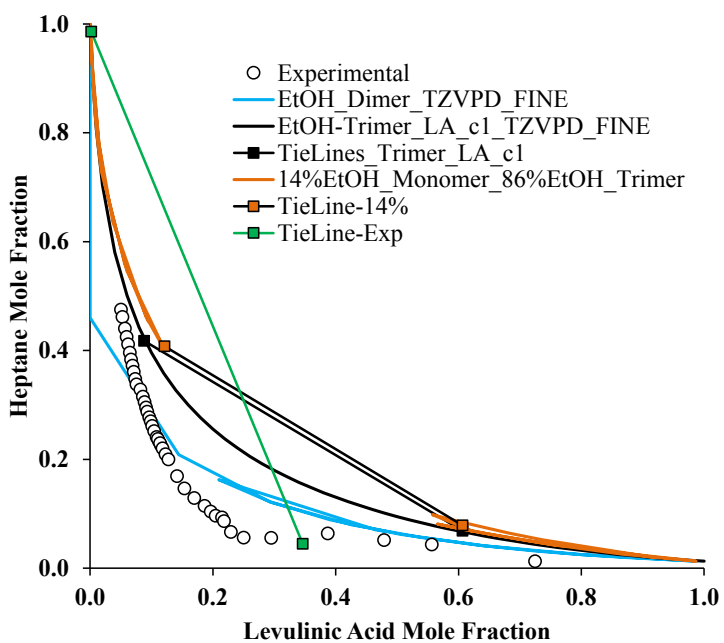
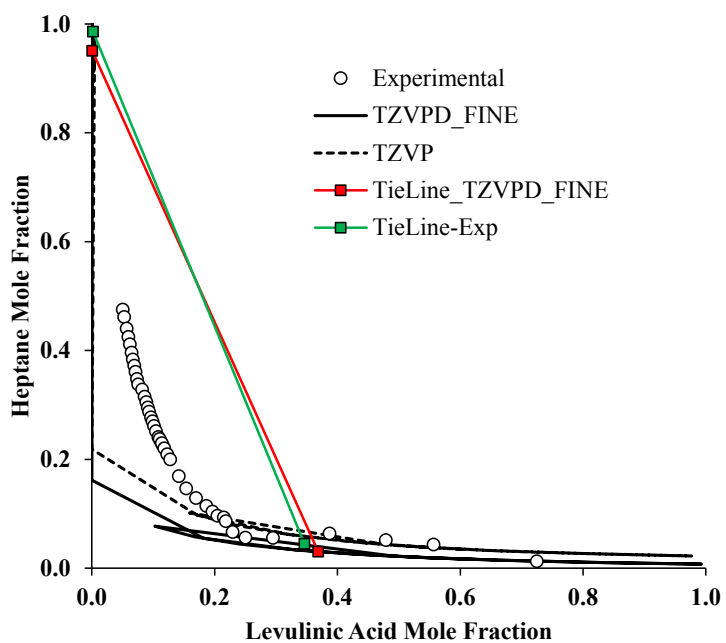


Figure S7. Experimental vs calculated binodal curves and tie lines by using ethanol monomer (A) and ethanol trimer approximation (B) with TZVP and TZVPD_FINE parametrizations at 25 °C in n-heptane/ethanol/levulinic acid OBS.

HPLC methodology

The quantification of composition of bottom phase was carried out using High-performance liquid chromatography (HPLC) with the following procedure. The samples were appropriately diluted and subsequently injected into an autosampler L-2200 (MiniSprin centrifuge, Hitachi, Ltd., Chiyoda, Japan) and passed through a Rezex ROA-Organic Acid H+ (8%) 300 × 7.8 mm ion-exchange column (Phenomenex, Torrance, CA, USA). The column temperature was maintained at 65 °C using an oven Gecko 2000 (CIL Cluzeau, Sainte-Foy-la-Grande, France). The detection of compounds was performed using a refractive index detector L-2490 (Hitachi, Chiyoda, Japan). For each injection, a volume of 50 µL was used, and the eluent employed was sulfuric acid (0.005 N), with a flow rate of 0.500 mL·min⁻¹, controlled by a pump L-2130 (Hitachi). To determine the concentration of compounds, a standard calibration curve was utilized. The composition of the upper phase was determined by mass balance.

Table S2. Exp. and calculated log P for system n-heptane-methanol at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|----------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-Acetonaphthone | -0.604 | -0.650 | -0.407 | -0.459 | -0.557 | -0.717 |
| 1-Bromododecane | 0.403 | 1.303 | 0.830 | 0.844 | 1.402 | 1.378 |
| 1-Bromonaphthalene | 0.062 | -0.098 | -0.080 | 0.066 | 0.241 | 0.209 |
| 1-Chloronaphthalene | 0.033 | 0.009 | -0.010 | 0.055 | 0.221 | 0.190 |
| 1-Naphthol | -1.106 | -2.269 | -0.756 | -0.896 | -1.291 | -1.753 |
| 1,2-Dichlorobenzene | -0.065 | -0.005 | -0.017 | -0.033 | 0.083 | 0.053 |
| 1,2-Dimethylbenzene | 0.177 | 0.911 | 0.587 | 0.573 | 0.920 | 0.915 |
| 1,4-Dichlorobenzene | 0.004 | -0.113 | -0.087 | 0.039 | 0.174 | 0.146 |
| 1,4-Dimethylbenzene | 0.184 | 0.293 | 0.169 | 0.177 | 0.356 | 0.336 |
| 2-Acetonaphthone | -0.566 | -0.762 | -0.468 | -0.480 | -0.594 | -0.770 |
| 2-Heptanone | -0.347 | -0.319 | -0.135 | -0.278 | -0.356 | -0.529 |
| 2-Hexanone | -0.423 | -0.471 | -0.237 | -0.383 | -0.514 | -0.682 |
| 2-Methoxynaphthalene | -0.131 | -0.218 | -0.168 | -0.138 | -0.061 | -0.113 |
| 2-Methylaniline | -0.838 | -1.249 | -0.795 | -0.760 | -0.996 | -1.167 |
| 2-Methylphenol | -1.013 | -1.278 | -0.491 | -0.710 | -1.069 | -1.442 |
| 2-Naphthol | -1.136 | -2.375 | -0.816 | -0.942 | -1.367 | -1.858 |
| 2-Nitrophenol | -0.563 | -0.683 | -0.461 | -0.465 | -0.542 | -0.602 |
| 2-Nonanone | -0.220 | -0.019 | 0.059 | -0.090 | -0.075 | -0.263 |
| 2-Octanone | -0.268 | -0.176 | -0.042 | -0.190 | -0.225 | -0.408 |
| 2-Pentanone | -0.495 | -0.624 | -0.333 | -0.475 | -0.651 | -0.814 |

| | | | | | | |
|------------------------|--------|--------|--------|--------|--------|--------|
| 2-Phenylethanol | -1.036 | -1.608 | -0.578 | -0.699 | -1.052 | -1.449 |
| 2,4-Dichlorophenol | -0.998 | -1.406 | -0.558 | -0.360 | -0.395 | -0.493 |
| 2,6-Dimethylphenol | -0.876 | -0.982 | -0.347 | -0.611 | -0.901 | -1.242 |
| 3-Methylaniline | -0.901 | -1.401 | -0.874 | -0.808 | -1.054 | -1.228 |
| 3-Methylphenol | -1.059 | -2.796 | -1.030 | -1.137 | -1.662 | -2.157 |
| 3,5-Dimethylphenol | -1.034 | -2.551 | -0.905 | -1.047 | -1.521 | -1.998 |
| 4-Acetylbiphenyl | -0.610 | -0.734 | -0.447 | -0.413 | -0.490 | -0.679 |
| 4-Chlorophenol | -1.137 | -3.266 | -1.181 | -1.170 | -1.711 | -2.251 |
| 4-Cyanophenol | -1.591 | -4.532 | -1.778 | -1.659 | -2.458 | -3.182 |
| 4-Hydroxybenzaldehyde | -1.524 | -4.459 | -1.683 | -1.624 | -2.454 | -3.232 |
| 4-Methylphenol | -1.122 | -2.783 | -1.036 | -1.130 | -1.650 | -2.140 |
| 4-Nitrotoluene | -0.478 | -0.390 | -0.281 | -0.559 | -0.669 | -0.763 |
| 4-Phenylphenol | -1.053 | -3.046 | -1.133 | -1.133 | -1.617 | -2.165 |
| Acetanilide | -1.334 | -2.239 | -1.251 | -1.291 | -1.851 | -2.269 |
| Acetophenone | -0.546 | -0.768 | -0.470 | -0.514 | -0.675 | -0.832 |
| Anisole | -0.140 | -0.237 | -0.178 | -0.171 | -0.147 | -0.191 |
| Anthraquinone | -0.425 | -0.689 | -0.460 | -0.393 | -0.453 | -0.590 |
| Benzamide | -1.535 | -3.423 | -1.885 | -1.715 | -2.469 | -2.970 |
| Benzophenone | -0.395 | -0.613 | -0.388 | -0.376 | -0.441 | -0.610 |
| Benzonitrile | -0.623 | -0.926 | -0.614 | -0.604 | -0.757 | -0.863 |
| Benzyl alcohol | -1.114 | -1.561 | -0.598 | -0.649 | -0.946 | -1.256 |
| Biphenyl | -0.018 | 0.608 | 0.378 | 0.421 | 0.737 | 0.715 |
| Butylbenzene | 0.264 | 0.557 | 0.343 | 0.353 | 0.632 | 0.610 |
| Chlorobenzene | 0.011 | -0.079 | -0.068 | -0.031 | 0.063 | 0.038 |
| Coumarin | -1.013 | -1.332 | -0.830 | -0.915 | -1.232 | -1.456 |
| Cyclohexanone | -0.607 | -0.680 | -0.361 | -0.467 | -0.662 | -0.851 |
| Dibutyl phthalate | -0.443 | 0.019 | 0.017 | -0.275 | -0.267 | -0.522 |
| N,N-Diethylcarbanilide | -0.605 | -0.582 | -0.237 | -0.263 | -0.323 | -0.618 |
| Diphenylamine | -0.631 | -0.836 | -0.537 | -0.508 | -0.544 | -0.647 |
| Ethylbenzene | 0.175 | 0.260 | 0.148 | 0.156 | 0.327 | 0.305 |
| Fluorene | -0.042 | -0.011 | -0.032 | 0.047 | 0.213 | 0.176 |
| Iodobenzene | 0.018 | -0.167 | -0.124 | 0.017 | 0.142 | 0.115 |
| Methyl decanoate | 0.079 | 0.513 | 0.355 | 0.317 | 0.554 | 0.416 |
| Methyl Octanoate | -0.028 | 0.216 | 0.160 | 0.120 | 0.248 | 0.114 |
| Naphthalene | -0.163 | 0.417 | 0.251 | 0.283 | 0.518 | 0.498 |
| Nicotinamide | -1.901 | -4.316 | -2.328 | -2.064 | -3.060 | -3.719 |
| Nitrobenzene | -0.476 | -0.004 | -0.032 | -0.305 | -0.331 | -0.402 |
| Nonanal | -0.087 | 0.162 | 0.128 | 0.043 | 0.154 | 0.028 |
| Nonan-1-ol | -0.546 | -1.241 | -0.331 | -0.486 | -0.731 | -1.147 |
| Octanal | -0.200 | 0.009 | 0.028 | -0.059 | -0.004 | -0.128 |
| Octan-1-ol | -0.470 | -1.382 | -0.425 | -0.573 | -0.860 | -1.264 |
| Phenanthrene | -0.005 | -0.137 | -0.112 | -0.009 | 0.152 | 0.108 |
| Phenol | -1.173 | -1.763 | -0.701 | -0.888 | -1.354 | -1.770 |
| Phenyl acetate | -0.534 | -0.780 | -0.517 | -0.524 | -0.660 | -0.778 |
| Phenylcyclohexane | 0.223 | 0.608 | 0.378 | 0.421 | 0.737 | 0.715 |
| Pyridine | -0.687 | -1.262 | -0.551 | -0.491 | -0.744 | -1.034 |
| p-Terphenyl | 0.067 | -0.003 | -0.029 | 0.132 | 0.389 | 0.340 |
| Toluene | 0.126 | 0.835 | 0.536 | 0.519 | 0.836 | 0.831 |
| Tribenzylamine | 0.187 | 0.416 | 0.244 | 0.406 | 0.808 | 0.761 |
| Triphenylene | -0.159 | -0.266 | -0.196 | -0.057 | 0.125 | 0.066 |
| Triphenylamine | 0.233 | 0.174 | 0.091 | 0.301 | 0.615 | 0.577 |
| Triphenylmethane | 0.140 | 1.838 | 1.199 | 1.340 | 2.086 | 2.085 |
| Valerophenone | -0.261 | -0.197 | -0.106 | -0.167 | -0.150 | -0.302 |

Table S3. Exp. and calculated log P for system n-hexane-acetonitrile at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|--------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-Acetonaphthone | -0.887 | -0.972 | -0.845 | -0.660 | -0.764 | -0.674 |
| 1-Bromododecane | 0.762 | 1.904 | 1.661 | 1.200 | 1.211 | 1.435 |
| 1-Bromohexane | 0.308 | 0.589 | 0.509 | 0.235 | 0.219 | 0.332 |
| 1-Bromonaphthalene | -0.025 | -0.484 | -0.382 | 0.132 | 0.103 | 0.226 |

| | | | | | | |
|--|--------|--------|--------|--------|--------|--------|
| 1-Chloronaphthalene | -0.002 | -0.244 | -0.181 | 0.132 | 0.104 | 0.223 |
| 1-Naphthol | -1.495 | -1.764 | -1.076 | -0.845 | -0.990 | -0.907 |
| 1-Nitronaphthalene | -0.906 | -1.214 | -1.044 | -0.880 | -0.988 | -0.904 |
| 1-Nitropropane | -1.136 | -0.999 | -0.884 | -1.201 | -1.306 | -1.303 |
| 1,2-Dichlorobenzene | -0.039 | -0.163 | -0.107 | -0.037 | -0.068 | 0.030 |
| 1,2-Dimethylbenzene | 0.113 | 1.562 | 1.370 | 1.003 | 1.034 | 1.184 |
| 1,3-Dichloro-1,1,3,3-tetramethyl-disiloxane | 1.134 | 0.532 | 0.456 | -0.234 | -0.279 | -0.171 |
| 1,3-Dinitrobenzene | -1.706 | -2.106 | -1.826 | -1.620 | -1.792 | -1.767 |
| 1,4-Dichlorobenzene | 0.060 | -0.288 | -0.208 | 0.071 | 0.047 | 0.144 |
| 1,4-Dimethylbenzene | 0.188 | 0.358 | 0.305 | 0.292 | 0.282 | 0.380 |
| 1,2,3-Trimethylbenzene | 0.292 | 1.719 | 1.507 | 1.108 | 1.142 | 1.306 |
| 2-Acetonaphthone | -1.142 | -1.062 | -0.925 | -0.716 | -0.829 | -0.739 |
| 2-Heptanone | -0.386 | 0.119 | 0.068 | -0.410 | -0.496 | -0.422 |
| 2-Hexanone | -0.509 | -0.117 | -0.137 | -0.581 | -0.674 | -0.623 |
| 2-Methoxynaphthalene | -0.495 | -0.613 | -0.529 | -0.233 | -0.286 | -0.191 |
| 2-Methylaniline | -1.185 | -1.425 | -1.211 | -0.803 | -0.927 | -0.899 |
| 2-Methylbenzothiazole | -0.699 | -0.744 | -0.634 | -0.189 | -0.250 | -0.161 |
| 2-Naphthol | -1.708 | -1.841 | -1.148 | -0.941 | -1.097 | -1.014 |
| 2-Nitroaniline | -1.796 | -2.493 | -2.073 | -1.659 | -1.835 | -1.814 |
| 2-Nitrophenol | -0.933 | -1.307 | -1.129 | -0.776 | -0.865 | -0.814 |
| 2-Nonanone | -0.150 | 0.564 | 0.459 | -0.083 | -0.159 | -0.037 |
| 2-Octanone | -0.308 | 0.334 | 0.257 | -0.254 | -0.335 | -0.237 |
| 2-Pentanone | -0.598 | -0.337 | -0.330 | -0.726 | -0.822 | -0.794 |
| 2-Phenylethanol | -1.347 | -0.487 | -0.274 | -0.312 | -0.407 | -0.313 |
| 2,2,4,4,6,6-Hexamethylcyclotrisilazane | 0.235 | 1.096 | 0.953 | 0.275 | 0.210 | 0.345 |
| 2,4-Dimethylaniline | -0.838 | -1.094 | -0.929 | -0.606 | -0.719 | -0.669 |
| 2,4,6,8-Tetramethyl-tetravinylcyclotetrasiloxane | 0.892 | 1.195 | 1.029 | 1.223 | 1.224 | 1.454 |
| 2,6-Dimethylphenol | -1.059 | -0.019 | 0.045 | -0.296 | -0.383 | -0.298 |
| 3-Aminopropyltriethoxysilane | -0.556 | -0.746 | -0.694 | -0.598 | -0.773 | -0.692 |
| 3-Methylaniline | -1.159 | -1.538 | -1.301 | -0.815 | -0.937 | -0.909 |
| 3,4-Dichloroaniline | -1.455 | -1.990 | -1.609 | -1.072 | -1.225 | -1.163 |
| 3,5-Dimethylphenol | -1.530 | -2.118 | -1.368 | -1.128 | -1.288 | -1.232 |
| 4-Acetylbiphenyl | -0.954 | -1.088 | -0.948 | -0.604 | -0.718 | -0.604 |
| 4-Chloroaniline | -1.447 | -1.986 | -1.645 | -1.073 | -1.220 | -1.187 |
| 4-Chlorophenol | -1.635 | -2.991 | -1.960 | -1.355 | -1.549 | -1.505 |
| 4-Cyanophenol | -2.286 | -4.370 | -3.022 | -2.139 | -2.445 | -2.428 |
| 4-Dimethylaminoazobenzene | -1.663 | -0.807 | -0.691 | -1.244 | -1.401 | -1.262 |
| 4-Methylphenol | -1.425 | -2.437 | -1.628 | -1.245 | -1.414 | -1.376 |
| 4-Nitrotoluene | -0.844 | -0.823 | -0.727 | -1.019 | -1.129 | -1.069 |
| 4-Phenylphenol | -1.712 | -2.962 | -2.015 | -1.251 | -1.450 | -1.371 |
| 8-Hydroxyquinoline | -0.966 | -1.072 | -0.899 | -0.473 | -0.537 | -0.457 |
| 9,10-Dimethylanthracene | -0.060 | -0.086 | -0.061 | 0.307 | 0.272 | 0.426 |
| Acetophenone | -0.853 | -0.960 | -0.849 | -0.792 | -0.894 | -0.848 |
| Aniline | -1.347 | 0.067 | 0.067 | 0.029 | -0.040 | 0.024 |
| Anisole | -0.395 | -0.514 | -0.455 | -0.302 | -0.346 | -0.289 |
| Anthraquinone | -0.806 | -1.310 | -1.134 | -0.462 | -0.552 | -0.443 |
| Azulene | -0.289 | -0.424 | -0.359 | -0.101 | -0.142 | -0.054 |
| Benzaldehyde | -0.852 | -1.092 | -0.958 | -0.797 | -0.892 | -0.852 |
| Benz[a]anthracene | -0.342 | -0.660 | -0.539 | 0.127 | 0.069 | 0.229 |
| Benzene | -0.071 | 1.248 | 1.094 | 0.802 | 0.828 | 0.951 |
| Benzidine | -1.873 | -3.601 | -3.036 | -2.000 | -2.244 | -2.236 |
| Benzophenone | -0.704 | -1.004 | -0.871 | -0.538 | -0.640 | -0.532 |
| Benzonitrile | -1.018 | -1.367 | -1.188 | -0.915 | -1.017 | -0.963 |
| Benzothiazole | -0.958 | -1.232 | -1.039 | -0.362 | -0.439 | -0.368 |
| Benzyl alcohol | -1.456 | -0.559 | -0.347 | -0.404 | -0.498 | -0.424 |
| Biphenyl | -0.159 | 0.855 | 0.747 | 0.707 | 0.706 | 0.861 |
| Borneol | -0.432 | -0.055 | 0.061 | -0.220 | -0.304 | -0.205 |

| | | | | | | |
|--------------------------------|--------|--------|--------|--------|--------|--------|
| Bromobenzene | -0.105 | 0.339 | 0.284 | -0.040 | -0.068 | 0.020 |
| Butyl acetate | -0.276 | -0.065 | -0.097 | -0.317 | -0.387 | -0.323 |
| Butylbenzene | 0.371 | 0.754 | 0.655 | 0.590 | 0.586 | 0.725 |
| Camphor | -0.337 | 0.318 | 0.236 | -0.331 | -0.415 | -0.335 |
| Chlorobenzene | -0.064 | -0.268 | -0.211 | -0.041 | -0.066 | 0.013 |
| Chrysene | -0.306 | -0.742 | -0.608 | 0.097 | 0.036 | 0.195 |
| Coumarin | -1.542 | -1.759 | -1.534 | -1.456 | -1.624 | -1.584 |
| Cyclohexanol | -0.865 | -0.761 | -0.532 | -0.586 | -0.691 | -0.643 |
| Cyclohexanone | -0.827 | -0.336 | -0.336 | -0.729 | -0.835 | -0.805 |
| Decamethylcyclopentasiloxane | 1.364 | 2.065 | 1.771 | 1.267 | 1.265 | 1.493 |
| Decamethyltetrasiloxane | 1.406 | 2.248 | 1.923 | 1.073 | 1.057 | 1.279 |
| Decan-1-ol | -0.199 | 0.271 | 0.390 | 0.201 | 0.123 | 0.287 |
| Diethoxydimethylsilane | 0.237 | 0.759 | 0.623 | 0.266 | 0.226 | 0.332 |
| N,N-Diethylcarbanilide | -0.629 | -0.282 | -0.256 | -0.204 | -0.326 | -0.167 |
| Dimethoxydimethylsilane | -0.101 | 0.152 | 0.090 | -0.058 | -0.106 | -0.046 |
| Dimethyl phthalate | -1.510 | -1.667 | -1.476 | -1.438 | -1.591 | -1.547 |
| Diphenylamine | -0.929 | -1.262 | -1.039 | -0.352 | -0.426 | -0.324 |
| Dodecamethylcyclohexasiloxane | 1.522 | 2.419 | 2.079 | 0.446 | 0.348 | 0.576 |
| Dodecamethylpentasiloxane | 1.633 | 2.125 | 1.786 | 1.160 | 1.127 | 1.380 |
| Dodecan-1-ol | 0.099 | 0.717 | 0.782 | 0.528 | 0.459 | 0.664 |
| Ethoxytrimethylsilane | 0.343 | 0.816 | 0.685 | 0.301 | 0.273 | 0.371 |
| Ethylbenzene | 0.156 | 0.302 | 0.260 | 0.281 | 0.269 | 0.367 |
| Ethyl propionate | -0.337 | -0.234 | -0.243 | -0.452 | -0.523 | -0.484 |
| Fluorene | -0.183 | -0.321 | -0.271 | 0.101 | 0.065 | 0.181 |
| Heptan-1-ol | -0.695 | -0.392 | -0.189 | -0.266 | -0.357 | -0.258 |
| Hexachlorobenzene | 0.372 | 0.838 | 0.769 | 0.951 | 0.964 | 1.141 |
| Hexamethylcyclotrisiloxane | 0.691 | 1.045 | 0.877 | 0.469 | 0.447 | 0.586 |
| Hexamethyldisilane | 1.042 | 1.901 | 1.657 | 1.023 | 1.047 | 1.205 |
| Hexamethyldisiloxane | 1.253 | 1.610 | 1.387 | 0.735 | 0.738 | 0.882 |
| Indole | -1.432 | -2.056 | -1.664 | -0.892 | -0.983 | -0.941 |
| Limonene | 0.678 | 1.122 | 0.969 | 0.718 | 0.726 | 0.864 |
| Linalool | -0.456 | 0.653 | 0.540 | 0.169 | 0.111 | 0.225 |
| Methyl benzoate | -0.638 | -0.770 | -0.678 | -0.472 | -0.544 | -0.476 |
| Methyl decanoate | 0.265 | 1.053 | 0.888 | 0.547 | 0.512 | 0.692 |
| Methyl hexanoate | -0.308 | 0.167 | 0.111 | -0.102 | -0.159 | -0.069 |
| Methyl nonanoate | 0.017 | 0.836 | 0.698 | 0.389 | 0.348 | 0.507 |
| Methyl Octanoate | -0.070 | 0.603 | 0.493 | 0.221 | 0.175 | 0.311 |
| Methyltriethoxysilane | 0.139 | 0.350 | 0.249 | -0.149 | -0.239 | -0.144 |
| Methyltrimethoxysilane | -0.381 | -0.190 | -0.213 | -0.315 | -0.379 | -0.328 |
| Naphthalene | -0.178 | 0.572 | 0.492 | 0.458 | 0.452 | 0.571 |
| Nicotinamide | -2.696 | -3.937 | -3.283 | -2.022 | -2.251 | -2.289 |
| Nitrobenzene | -0.923 | -0.085 | -0.110 | -0.686 | -0.763 | -0.709 |
| Nonan-1-ol | -0.423 | 0.062 | 0.207 | 0.055 | -0.027 | 0.116 |
| Octamethylcyclotetrasiloxane | 1.176 | 1.808 | 1.549 | 0.847 | 0.836 | 1.023 |
| Octamethyltrisiloxane | 1.164 | 1.815 | 1.549 | 0.739 | 0.717 | 0.896 |
| Octane | 1.083 | 1.978 | 1.731 | 1.251 | 1.291 | 1.473 |
| Octan-1-ol | -0.470 | -0.158 | 0.014 | -0.100 | -0.186 | -0.064 |
| Octanophenone | -0.052 | 0.507 | 0.435 | 0.267 | 0.204 | 0.385 |
| Perylene | -0.656 | -0.772 | -0.627 | 0.146 | 0.083 | 0.255 |
| Phenanthrene | -0.254 | -0.549 | -0.453 | 0.069 | 0.024 | 0.150 |
| Phenol | -1.602 | -0.761 | -0.532 | -0.586 | -0.691 | -0.643 |
| Phenylcyclohexane | 0.433 | 0.855 | 0.747 | 0.707 | 0.706 | 0.861 |
| alpha-Pinene | 0.846 | 1.505 | 1.317 | 0.963 | 0.987 | 1.140 |
| beta-Pinene | 0.854 | 1.325 | 1.152 | 0.785 | 0.799 | 0.937 |
| Phenylcyclohexane | 0.433 | 0.855 | 0.747 | 0.707 | 0.706 | 0.861 |
| n-Propylbenzene | 0.258 | 0.527 | 0.456 | 0.436 | 0.428 | 0.546 |
| p-Terphenyl | -0.186 | -0.541 | -0.445 | 0.260 | 0.210 | 0.379 |
| Terpinen-4-ol | -0.432 | 0.653 | 0.568 | 0.173 | 0.120 | 0.235 |
| Tetraethylorthosilicate | 0.102 | -0.059 | -0.128 | 0.400 | 0.364 | 0.521 |
| Tetramethyldisiloxane-1,3-diol | -1.232 | -2.462 | -1.772 | -2.090 | -2.329 | -2.321 |

| | | | | | | |
|--------------------------|--------|--------|--------|--------|--------|--------|
| Tetramethylorthosilicate | -0.588 | -0.209 | -0.226 | -0.218 | -0.270 | -0.209 |
| Tetramethylsilane | 0.779 | 1.310 | 1.140 | 0.613 | 0.628 | 0.735 |
| Toluene | 0.053 | 1.444 | 1.266 | 0.915 | 0.944 | 1.084 |
| Tribenzylamine | 0.108 | 0.142 | 0.137 | 0.714 | 0.678 | 0.894 |
| Triphenylene | -0.407 | -0.823 | -0.675 | 0.069 | 0.004 | 0.161 |
| Triphenylmethane | 0.083 | 3.026 | 2.662 | 2.234 | 2.299 | 2.601 |
| Valerophenone | -0.445 | -0.150 | -0.140 | -0.230 | -0.309 | -0.193 |
| Vinyltrimethoxysilane | -0.354 | -0.448 | -0.434 | -0.403 | -0.482 | -0.428 |

Table S4. Experimental and calculated log P for system n-heptane-N,N-dimethylformamide at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_MS | TZVPDFINE_EXP_MS | TZVPDFINE_PRED_FINE_MS | TZVPDFINE_PRED_TZVP_MS |
|---|--------|---------|-------------|------------------|------------------------|------------------------|
| 1-Acetonaphthone | -1.234 | -1.511 | -1.345 | -1.249 | -1.237 | -0.658 |
| 1-Bromododecane | 0.495 | 0.107 | 0.114 | 0.761 | 0.932 | 0.332 |
| 1-Bromonaphthalene | -0.522 | -1.156 | -0.998 | -0.530 | -0.480 | -0.318 |
| 1-Chloronaphthalene | -0.544 | -0.993 | -0.858 | -0.497 | -0.448 | -0.299 |
| 1-Nitronaphthalene | -1.349 | -1.751 | -1.550 | -1.564 | -1.565 | -0.824 |
| 1,2-Dichlorobenzene | -0.384 | -0.867 | -0.745 | -0.551 | -0.513 | -0.318 |
| 1,2-Dimethylbenzene | -0.006 | 0.416 | 0.390 | 0.740 | 0.849 | 0.355 |
| 1,3-Dichloro-1,1,3,3-tetramethyldisiloxane | 1.065 | -0.549 | -0.483 | -0.493 | -0.428 | -0.311 |
| 1,4-Dimethylbenzene | -0.012 | -0.369 | -0.322 | -0.009 | 0.047 | -0.028 |
| 2-Acetonaphthone | -1.311 | -1.587 | -1.416 | -1.302 | -1.290 | -0.684 |
| 2-Heptanone | -0.339 | -0.538 | -0.503 | -0.568 | -0.530 | -0.298 |
| 2-Methoxynaphthalene | -0.887 | -1.268 | -1.121 | -0.749 | -0.719 | -0.411 |
| 2-Methylphenol | -1.682 | -1.546 | -1.202 | -1.139 | -1.132 | -0.498 |
| 2-Nonanone | -0.162 | -0.395 | -0.372 | -0.322 | -0.246 | -0.187 |
| 2-Octanone | -0.289 | -0.474 | -0.444 | -0.458 | -0.401 | -0.249 |
| 2-Phenylethanol | -1.623 | -1.955 | -1.454 | -1.136 | -1.115 | -0.484 |
| 2,2,4,4,6,6-Hexamethylcyclotrisilazane | -0.082 | -0.502 | -0.441 | -0.197 | -0.110 | -0.135 |
| 2,4,6,8-Tetramethyl-tetramethylcyclotetrasiloxane | 0.699 | -0.505 | -0.439 | 0.734 | 0.928 | 0.284 |
| 2,6-Dimethylphenol | -1.445 | -1.246 | -0.980 | -1.028 | -1.006 | -0.451 |
| 3-Aminopropyltriethoxysilane | -0.470 | -1.500 | -1.407 | -0.888 | -0.854 | -0.383 |
| 4-Acetylbiphenyl | -1.342 | -1.717 | -1.531 | -1.310 | -1.285 | -0.696 |
| 4-Methylphenol | -1.775 | -3.971 | -2.631 | -2.060 | -2.132 | -0.884 |
| 4-Nitrotoluene | -1.045 | -1.274 | -1.138 | -1.464 | -1.469 | -0.779 |
| Acetophenone | -1.069 | -1.281 | -1.151 | -1.133 | -1.138 | -0.587 |
| Anisole | -0.546 | -0.969 | -0.862 | -0.595 | -0.581 | -0.320 |
| Benzaldehyde | -1.161 | -1.340 | -1.200 | -1.130 | -1.139 | -0.586 |
| Benzene | -0.193 | 0.325 | 0.308 | 0.579 | 0.666 | 0.274 |
| Benzonitrile | -1.185 | -1.643 | -1.466 | -1.396 | -1.408 | -0.727 |
| Benzyl alcohol | -1.824 | -1.903 | -1.428 | -1.097 | -1.085 | -0.478 |
| Biphenyl | -0.545 | -0.236 | -0.196 | 0.274 | 0.374 | 0.109 |
| Butylbenzene | 0.148 | -0.263 | -0.223 | 0.194 | 0.282 | 0.072 |
| Chlorobenzene | -0.312 | -0.837 | -0.725 | -0.456 | -0.427 | -0.267 |
| Chrysene | -1.312 | -1.715 | -1.498 | -0.889 | -0.832 | -0.477 |
| Decamethylcyclopentasiloxane | 1.301 | 0.110 | 0.101 | 1.010 | 1.219 | 0.449 |
| Decamethyltetrasiloxane | 1.378 | 0.230 | 0.200 | 0.851 | 1.047 | 0.387 |
| Decan-1-ol | -0.688 | -1.721 | -1.237 | -0.736 | -0.652 | -0.294 |
| Dibenzyl ether | -0.770 | -1.524 | -1.364 | -1.015 | -0.979 | -0.512 |

| | | | | | | |
|--------------------------------|--------|--------|--------|--------|--------|--------|
| Diethoxydimethylsilane | 0.353 | -0.174 | -0.171 | 0.107 | 0.184 | 0.049 |
| N,N-Diethylcarbanilide | -1.127 | -1.246 | -1.117 | -0.896 | -0.817 | -0.494 |
| Dimethoxydimethylsilane | 0.085 | -0.423 | -0.400 | -0.120 | -0.080 | -0.055 |
| Diphenylamine | -1.558 | -2.307 | -2.001 | -1.407 | -1.398 | -0.737 |
| Dodecamethylcyclohexasiloxane | 1.525 | 0.148 | 0.138 | 0.205 | 0.402 | 0.089 |
| Dodecamethylpentasiloxane | 1.524 | -0.069 | -0.095 | 0.919 | 1.149 | 0.416 |
| Ethoxytrimethylsilane | 0.596 | -0.050 | -0.054 | 0.161 | 0.233 | 0.074 |
| Ethylbenzene | -0.013 | -0.414 | -0.360 | -0.041 | 0.013 | -0.040 |
| Fluorene | -0.589 | -1.074 | -0.943 | -0.490 | -0.441 | -0.280 |
| Heptan-1-ol | -0.746 | -1.932 | -1.428 | -1.084 | -1.059 | -0.456 |
| Hexachlorobenzene | -0.307 | -0.123 | -0.072 | 0.438 | 0.549 | 0.191 |
| Hexamethylcyclotrisiloxane | 0.708 | -0.207 | -0.192 | 0.305 | 0.418 | 0.127 |
| Hexamethylidisilane | 0.968 | 0.458 | 0.426 | 0.843 | 0.968 | 0.409 |
| Hexamethyldisiloxane | 0.997 | 0.254 | 0.231 | 0.578 | 0.694 | 0.269 |
| Iodobenzene | -0.422 | -1.049 | -0.907 | -0.505 | -0.471 | -0.298 |
| Methyl decanoate | 0.185 | -0.261 | -0.244 | 0.189 | 0.318 | 0.054 |
| Methyl Octanoate | -0.025 | -0.409 | -0.379 | -0.066 | 0.022 | -0.060 |
| Methyltriethoxysilane | 0.301 | -0.486 | -0.470 | -0.309 | -0.247 | -0.147 |
| Methyltrimethoxysilane | -0.196 | -0.691 | -0.641 | -0.385 | -0.358 | -0.191 |
| Naphthalene | -0.548 | -0.283 | -0.244 | 0.114 | 0.188 | 0.030 |
| Nicotinamide | -3.100 | -4.708 | -4.064 | -3.249 | -3.362 | -1.645 |
| Nonan-1-ol | -0.601 | -1.779 | -1.292 | -0.850 | -0.785 | -0.349 |
| Octamethylcyclotetrasiloxane | 1.291 | 0.064 | 0.060 | 0.625 | 0.788 | 0.265 |
| Octamethyltrisiloxane | 1.160 | 0.164 | 0.138 | 0.540 | 0.686 | 0.246 |
| Octan-1-ol | -0.679 | -1.851 | -1.359 | -0.966 | -0.921 | -0.404 |
| Octanophenone | -0.371 | -0.729 | -0.648 | -0.346 | -0.238 | -0.225 |
| Perylene | -1.477 | -1.784 | -1.556 | -0.942 | -0.880 | -0.506 |
| Phenanthrene | -0.872 | -1.331 | -1.163 | -0.665 | -0.618 | -0.363 |
| Phenylcyclohexane | 0.047 | -0.236 | -0.196 | 0.274 | 0.374 | 0.109 |
| Phenyl acetate | -1.068 | -1.585 | -1.423 | -1.197 | -1.210 | -0.618 |
| Phenylcyclohexane | 0.047 | -0.236 | -0.196 | 0.274 | 0.374 | 0.109 |
| Tetraethylorthosilicate | 0.237 | -0.783 | -0.751 | 0.139 | 0.252 | 0.037 |
| Tetramethyldisiloxane-1,3-diol | -1.802 | -4.476 | -3.282 | -3.337 | -3.465 | -1.399 |
| Tetramethylorthosilicate | -0.375 | -0.761 | -0.698 | -0.322 | -0.290 | -0.164 |
| Tetramethylsilane | 0.835 | 0.283 | 0.265 | 0.481 | 0.562 | 0.227 |
| Toluene | -0.062 | 0.385 | 0.362 | 0.675 | 0.775 | 0.321 |
| Tribenzylamine | -0.583 | -1.200 | -1.047 | -0.204 | -0.075 | -0.165 |
| Triphenylamine | -0.445 | -1.297 | -1.128 | -0.374 | -0.281 | -0.257 |
| Triphenylmethane | -0.651 | 0.863 | 0.806 | 1.702 | 1.936 | 0.843 |
| Valerophenone | -0.585 | -0.942 | -0.843 | -0.717 | -0.667 | -0.392 |
| Vinyltrimethoxysilane | -0.226 | -0.888 | -0.820 | -0.514 | -0.489 | -0.255 |

Table S5. Experimental and calculated log P for system n-heptane-trifluoroethanol at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_MS | TZVPDFINE_EXP_MS | TZVPDFINE_P_RED_FINE_MS | TZVPDFINE_P_RED_TZVP_MS |
|------------------|--------|---------|-------------|------------------|-------------------------|-------------------------|
| 1-Acetonaphthone | -0.753 | -1.102 | -0.823 | -0.659 | -0.742 | -0.850 |
| 1-Bromododecane | 1.410 | 2.077 | 1.988 | 1.636 | 1.589 | 1.645 |

| | | | | | | |
|--|--------|--------|--------|--------|--------|--------|
| 1-Bromohexane | 0.875 | 0.961 | 0.921 | 0.569 | 0.542 | 0.565 |
| 1-Bromonaphthalene | 0.927 | 0.696 | 0.670 | 0.757 | 0.729 | 0.756 |
| 1-Bromooctane | 1.183 | 1.335 | 1.279 | 0.921 | 0.888 | 0.922 |
| 1-Bromopentane | 0.343 | 0.769 | 0.737 | 0.394 | 0.371 | 0.388 |
| 1-Chloronaphthalene | 0.896 | 0.563 | 0.542 | 0.714 | 0.688 | 0.714 |
| 1-Hydroxyanthraquinone | -0.612 | -0.907 | -0.781 | -0.578 | -0.644 | -0.704 |
| 1-Nitronaphthalene | -0.360 | -0.563 | -0.507 | -0.603 | -0.656 | -0.709 |
| 1-Nitropropane | -1.180 | -0.844 | -0.779 | -1.026 | -1.060 | -1.116 |
| 1,2-Dichlorobenzene | 0.683 | 0.565 | 0.543 | 0.540 | 0.518 | 0.538 |
| 1,2-Dimethylbenzene | 0.537 | 1.356 | 1.295 | 1.203 | 1.179 | 1.217 |
| 1,3-Dinitrobenzene | -1.420 | -1.257 | -1.173 | -1.309 | -1.350 | -1.403 |
| 1,4-Dimethylbenzene | 0.602 | 0.537 | 0.517 | 0.597 | 0.575 | 0.596 |
| 1,2,4,5-Tetrachlorobenzene | 1.351 | 1.034 | 0.992 | 1.167 | 1.138 | 1.177 |
| 2-Acetonaphthone | -0.960 | -1.382 | -1.033 | -0.760 | -0.842 | -0.946 |
| 2-Heptanone | -0.984 | -1.444 | -0.913 | -0.874 | -0.952 | -1.057 |
| 2-Hexanone | -1.144 | -1.630 | -1.098 | -1.027 | -1.101 | -1.208 |
| 2-Methoxynaphthalene | 0.163 | -0.010 | 0.010 | 0.144 | 0.109 | 0.109 |
| 2-Methylaniline | -1.130 | -1.024 | -0.813 | -0.918 | -0.973 | -1.052 |
| 2-Methylbenzothiazole | -0.746 | -1.064 | -0.674 | -0.371 | -0.461 | -0.602 |
| 2-Methylphenol | -0.857 | -1.557 | -0.762 | -1.328 | -1.460 | -1.701 |
| 2-Naphthol | -1.101 | -1.029 | -0.766 | -0.870 | -0.932 | -1.000 |
| 2-Nitrophenol | -0.704 | -0.764 | -0.700 | -0.578 | -0.614 | -0.646 |
| 2-Nonanone | -0.409 | -1.051 | -0.548 | -0.642 | -0.735 | -0.848 |
| 2-Octanone | -0.845 | -1.253 | -0.731 | -0.784 | -0.871 | -0.985 |
| 2-Phenylacetamide | -3.162 | -4.629 | -2.937 | -2.583 | -2.750 | -3.111 |
| 2,2,4,4,6,6-Hexamethylcyclotrisilazane | -0.455 | 0.331 | 0.577 | -0.063 | -0.140 | -0.199 |
| 2,4-Dimethylaniline | -1.155 | -0.927 | -0.645 | -0.754 | -0.825 | -0.930 |
| 2,4,6,8-Tetramethyl-tetravinylcyclotetrasiloxane | 1.227 | 1.185 | 1.166 | 1.549 | 1.496 | 1.547 |
| 2,5-Dichloroaniline | 0.735 | -0.286 | -0.238 | -0.177 | -0.209 | -0.224 |
| 3-Aminopropyltriethoxysilane | -2.337 | -6.290 | -2.801 | -2.595 | -2.768 | -3.106 |
| 3-Bromophenol | -0.904 | -1.083 | -0.788 | -1.030 | -1.082 | -1.148 |
| 3-Methylaniline | -1.269 | -1.172 | -0.895 | -0.950 | -1.011 | -1.103 |
| 3-Methylphenol | -1.170 | -1.377 | -1.093 | -1.169 | -1.221 | -1.292 |
| 3,5-Dinitroaniline | -2.367 | -2.077 | -1.924 | -2.357 | -2.432 | -2.579 |
| 4-Acetylbiphenyl | -0.718 | -1.358 | -0.986 | -0.651 | -0.742 | -0.854 |
| 4-Bromoacetanilide | -2.185 | -2.143 | -1.520 | -1.570 | -1.678 | -1.871 |
| 4-Bromophenol | -0.973 | -1.173 | -0.877 | -1.001 | -1.050 | -1.109 |
| 4-Chlorophenol | -0.917 | -1.337 | -1.031 | -1.068 | -1.116 | -1.178 |
| 4-Chloro-2-nitroaniline | -1.069 | -1.577 | -1.393 | -1.449 | -1.520 | -1.641 |
| 4-Cyanophenol | -1.976 | -3.180 | -2.550 | -2.395 | -2.500 | -2.707 |
| 4-Dimethylaminoazobenzene | -2.857 | -0.264 | -0.164 | -0.697 | -0.768 | -0.823 |
| 4-Fluoroaniline | -1.422 | -1.433 | -1.151 | -1.279 | -1.335 | -1.432 |
| 4-Hydroxybenzyl alcohol | -2.987 | -3.972 | -2.913 | -3.114 | -3.246 | -3.510 |
| 4-Methylaniline | -1.384 | -1.238 | -0.903 | -0.908 | -0.973 | -1.075 |
| 4-Methylphenol | -1.151 | -1.386 | -1.100 | -1.144 | -1.196 | -1.266 |
| 4-Nitrobenzyl alcohol | -2.183 | -2.801 | -2.258 | -2.657 | -2.753 | -2.932 |
| 4-Nitrotoluene | -0.674 | -0.659 | -0.588 | -0.850 | -0.901 | -0.968 |
| 4-Phenylphenol | -0.945 | -1.290 | -1.008 | -0.937 | -0.998 | -1.060 |
| 8-Hydroxyquinoline | -0.619 | -0.464 | -0.396 | -0.301 | -0.342 | -0.371 |
| 9,10-Dimethylanthracene | 1.083 | 0.665 | 0.642 | 0.927 | 0.892 | 0.924 |
| Acetophenone | -1.071 | -1.542 | -1.181 | -0.937 | -1.007 | -1.112 |
| Aniline | -1.315 | -2.577 | -0.505 | -0.605 | -0.724 | -0.978 |
| Anise Alcohol | -2.049 | -2.605 | -1.819 | -1.985 | -2.095 | -2.294 |
| Anisole | -0.140 | -0.216 | -0.182 | -0.075 | -0.103 | -0.113 |
| Anthraquinone | -0.416 | -1.215 | -1.042 | -0.739 | -0.809 | -0.885 |
| Azulene | 0.401 | 0.219 | 0.215 | 0.361 | 0.337 | 0.352 |

| | | | | | | |
|-------------------------------|--------|--------|--------|--------|--------|--------|
| Benzaldehyde | -0.978 | -1.410 | -1.145 | -0.927 | -0.989 | -1.082 |
| Benz[a]anthracene | 1.205 | 0.527 | 0.512 | 0.858 | 0.819 | 0.849 |
| Benzene | 0.319 | 1.075 | 1.026 | 0.951 | 0.932 | 0.962 |
| Benzidine | -2.724 | -2.506 | -2.036 | -2.252 | -2.364 | -2.563 |
| Benzo[ghi]perylene | 1.442 | 0.679 | 0.656 | 1.064 | 1.020 | 1.056 |
| Benzophenone | -0.637 | -1.117 | -0.855 | -0.514 | -0.590 | -0.673 |
| Benzonitrile | -1.153 | -1.252 | -1.067 | -0.950 | -1.008 | -1.098 |
| Benzo[e]pyrene | 1.266 | 0.567 | 0.550 | 0.944 | 0.903 | 0.935 |
| Benzothiazole | -0.898 | -1.341 | -0.936 | -0.506 | -0.593 | -0.733 |
| Benzyl alcohol | -1.442 | -1.670 | -0.864 | -1.264 | -1.387 | -1.601 |
| Benzyl salicylate | 0.144 | -0.300 | -0.227 | -0.149 | -0.215 | -0.255 |
| Biphenyl | 0.671 | 0.994 | 0.953 | 1.056 | 1.025 | 1.061 |
| Borneol | -0.703 | -0.957 | -0.354 | -0.772 | -0.879 | -1.040 |
| Butylbenzene | 0.913 | 0.901 | 0.864 | 0.918 | 0.890 | 0.921 |
| Butyl stearate | 1.685 | 1.891 | 2.070 | 1.780 | 1.655 | 1.640 |
| Camphor | -0.922 | -1.263 | -0.815 | -0.866 | -0.952 | -1.073 |
| Carvone | -0.840 | -1.841 | -1.194 | -1.186 | -1.285 | -1.438 |
| Chlorobenzene | 0.564 | 0.359 | 0.346 | 0.421 | 0.402 | 0.419 |
| Chrysene | 1.262 | 0.491 | 0.477 | 0.848 | 0.809 | 0.838 |
| Cyclohexanol | -1.335 | -2.100 | -1.145 | -1.597 | -1.728 | -1.979 |
| Cyclohexanone | -1.329 | -2.054 | -1.447 | -1.434 | -1.525 | -1.682 |
| Decamethylcyclopentasiloxane | 1.517 | 1.321 | 1.317 | 1.369 | 1.308 | 1.346 |
| Decamethyltetrasiloxane | 1.508 | 0.853 | 1.088 | 1.196 | 1.134 | 1.163 |
| Decan-1-ol | -0.366 | -1.158 | -0.257 | -0.816 | -0.964 | -1.189 |
| Dibenzyl ether | -0.634 | -1.027 | -0.628 | -0.116 | -0.180 | -0.219 |
| Dibutyl phthalate | -1.080 | -1.000 | -0.710 | -0.836 | -0.952 | -1.086 |
| Dicyclohexylamine | 0.184 | -0.398 | 0.852 | 0.538 | 0.407 | 0.201 |
| Diethoxydimethylsilane | -0.798 | -0.930 | -0.401 | -0.559 | -0.632 | -0.706 |
| Diethyl adipate | -1.724 | -2.773 | -2.157 | -1.918 | -2.000 | -2.101 |
| Diethyl phthalate | -1.874 | -1.824 | -1.506 | -1.405 | -1.503 | -1.644 |
| Di-2-ethylhexyl phthalate | -0.775 | 0.123 | 0.401 | 0.229 | 0.085 | -0.020 |
| Diisobutyl phthalate | -1.049 | -0.984 | -0.700 | -0.970 | -1.090 | -1.234 |
| Dimethoxydimethylsilane | -0.580 | -1.567 | -0.942 | -1.140 | -1.219 | -1.333 |
| Dimethyl phthalate | -2.045 | -2.104 | -1.805 | -1.426 | -1.504 | -1.624 |
| Diocetyl phthalate | -0.341 | 0.417 | 0.664 | 0.190 | 0.030 | -0.097 |
| Diphenyl ether | 0.603 | 0.324 | 0.319 | 0.550 | 0.517 | 0.534 |
| Dodecamethylcyclohexasiloxane | 1.688 | 1.646 | 1.635 | 0.748 | 0.659 | 0.646 |
| Dodecamethylpentasiloxane | 1.742 | -0.802 | 0.052 | 1.245 | 1.168 | 1.195 |
| Dodecan-1-ol | 0.130 | -0.776 | 0.110 | -0.526 | -0.687 | -0.916 |
| Ethanol | -1.649 | -2.856 | -1.763 | -1.995 | -2.100 | -2.319 |
| Ethoxytrimethylsilane | -0.277 | -0.651 | -0.085 | -0.176 | -0.241 | -0.306 |
| Ethylbenzene | 0.601 | 0.525 | 0.505 | 0.578 | 0.556 | 0.577 |
| Eugenol | -0.564 | -0.514 | -0.410 | -0.459 | -0.507 | -0.541 |
| Fluorene | 0.703 | 0.371 | 0.361 | 0.616 | 0.586 | 0.609 |
| Hexachlorobenzene | 1.626 | 1.451 | 1.388 | 1.623 | 1.588 | 1.640 |
| Hexamethylcyclotrisiloxane | 0.610 | 0.210 | 0.307 | 0.033 | -0.022 | -0.039 |
| Hexamethyldisilane | 1.297 | 1.675 | 1.600 | 1.203 | 1.174 | 1.214 |
| Hexamethyldisiloxane | 1.145 | 0.965 | 0.988 | 0.833 | 0.797 | 0.818 |
| Iodobenzene | 0.854 | -0.039 | -0.034 | 0.558 | 0.536 | 0.557 |
| Limonene | 1.231 | 1.048 | 1.004 | 0.885 | 0.855 | 0.883 |
| Linalool | -0.814 | -0.940 | -0.211 | -0.684 | -0.801 | -0.974 |
| Methyl decanoate | -0.011 | -0.193 | 0.059 | 0.121 | 0.047 | 0.004 |
| Methyl hexanoate | -0.630 | -0.920 | -0.649 | -0.424 | -0.478 | -0.528 |
| Methyl nonanoate | -0.143 | -0.364 | -0.110 | -0.025 | -0.094 | -0.136 |
| Methyl Octanoate | -0.321 | -0.572 | -0.304 | -0.182 | -0.247 | -0.294 |
| Methyltriethoxysilane | -0.861 | -2.349 | -1.284 | -1.015 | -1.094 | -1.182 |
| Methyltrimethoxysilane | -1.412 | -1.543 | -1.145 | -1.017 | -1.076 | -1.149 |
| Naphthalene | 0.550 | 0.685 | 0.658 | 0.777 | 0.752 | 0.779 |
| Nicotinamide | -3.352 | -5.625 | -3.885 | -3.658 | -3.857 | -4.313 |
| Octamethylcyclotetrasiloxane | 1.330 | 1.123 | 1.125 | 0.702 | 0.644 | 0.655 |

| | | | | | | |
|---------------------------|--------|--------|--------|--------|--------|--------|
| Octamethyltrisiloxane | 1.314 | 0.347 | 0.684 | 0.895 | 0.843 | 0.860 |
| Octan-1-ol | -0.706 | -1.526 | -0.601 | -1.139 | -1.279 | -1.509 |
| Octanophenone | -0.008 | -0.196 | 0.058 | 0.188 | 0.104 | 0.045 |
| Perylene | 0.917 | 0.553 | 0.536 | 0.935 | 0.894 | 0.926 |
| Phenanthrene | 0.806 | 0.390 | 0.379 | 0.673 | 0.641 | 0.665 |
| Phenol | -1.440 | -2.100 | -1.145 | -1.597 | -1.728 | -1.979 |
| Phenylcyclohexane | 0.959 | 0.994 | 0.953 | 1.056 | 1.025 | 1.061 |
| Phthalimide | -2.136 | -2.781 | -2.448 | -2.087 | -2.159 | -2.287 |
| alpha-Pinene | 1.140 | 1.365 | 1.305 | 1.149 | 1.122 | 1.158 |
| beta-Pinene | 1.151 | 1.170 | 1.120 | 0.901 | 0.871 | 0.898 |
| Phenyl acetate | -1.092 | -1.397 | -1.184 | -0.767 | -0.822 | -0.895 |
| Phenyl benzoate | -0.428 | -0.699 | -0.556 | -0.186 | -0.253 | -0.313 |
| Phenylcyclohexane | 0.959 | 0.994 | 0.953 | 1.056 | 1.025 | 1.061 |
| Pyridine | -1.570 | -2.168 | -1.116 | -0.965 | -1.072 | -1.308 |
| Styrene | 0.484 | 0.254 | 0.247 | 0.385 | 0.364 | 0.379 |
| p-Terphenyl | 0.437 | 0.582 | 0.565 | 0.979 | 0.938 | 0.972 |
| Terpinen-4-ol | -0.531 | -0.518 | -0.005 | -0.453 | -0.561 | -0.721 |
| Tetraethylorthosilicate | -0.876 | -3.205 | -2.155 | -0.173 | -0.241 | -0.280 |
| Tetramethylorthosilicate | -1.418 | -0.992 | -0.819 | -0.820 | -0.874 | -0.932 |
| Tetramethylsilane | 0.910 | 1.131 | 1.080 | 0.761 | 0.741 | 0.767 |
| Toluene | 0.455 | 1.242 | 1.186 | 1.085 | 1.063 | 1.098 |
| Tribenzylamine | 1.038 | 1.004 | 0.968 | 1.351 | 1.301 | 1.348 |
| Tri- <i>n</i> -butylamine | 0.138 | 0.846 | 1.955 | 1.388 | 1.307 | 1.280 |
| Tri- <i>n</i> -butyrin | -2.099 | -2.728 | -2.154 | -2.026 | -2.122 | -2.228 |
| Triphenylene | 1.135 | 0.458 | 0.446 | 0.836 | 0.797 | 0.826 |
| Triphenylamine | 1.189 | 0.768 | 0.741 | 1.142 | 1.102 | 1.142 |
| Triphenylmethane | 0.986 | 2.652 | 2.534 | 2.589 | 2.542 | 2.621 |
| Valerophenone | -0.528 | -0.748 | -0.471 | -0.276 | -0.348 | -0.417 |
| Vanillin | -2.125 | -2.518 | -2.002 | -1.677 | -1.767 | -1.923 |
| Vinyltrimethoxysilane | -1.136 | -2.168 | -1.429 | -0.870 | -0.926 | -0.989 |
| Vinyltrimethylsilane | 0.965 | 1.003 | 0.959 | 0.694 | 0.672 | 0.697 |

Table S6. Experimental and calculated log P for system n-heptane-propylene carbonate at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|-----------------------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-(1-naphthalenyl)-ethanone | -0.909 | -0.887 | -0.897 | -0.852 | -0.862 | -0.795 |
| 1-bromododecane | 1.275 | 1.505 | 1.447 | 1.608 | 1.582 | 1.606 |
| 1-bromohexane | 0.706 | 0.429 | 0.402 | 0.439 | 0.426 | 0.449 |
| 1-bromonaphthalene | 0.089 | -0.347 | -0.356 | 0.100 | 0.087 | 0.122 |
| 1-bromooctane | 1.056 | 0.788 | 0.751 | 0.832 | 0.815 | 0.838 |
| 1-chloronaphthalene | 0.167 | -0.199 | -0.211 | 0.116 | 0.104 | 0.137 |
| 1-methyl-tetralin | 0.066 | 0.538 | 0.508 | 0.721 | 0.707 | 0.728 |
| 5,6,7,8-tetrahydro-1-naphthalenol | -2.426 | -1.632 | -1.618 | -1.166 | -1.176 | -0.929 |
| 1-nitro-naphthalene | -0.983 | -1.037 | -1.041 | -1.137 | -1.145 | -1.072 |
| a-methylcyclohexanemethanol | -1.171 | -0.127 | -0.153 | -0.196 | -0.207 | -0.064 |
| 1,3-dinitrobenzene | -1.991 | -1.684 | -1.678 | -2.079 | -2.082 | -1.971 |
| 1,2,4,5-tetrachlorobenzene | 0.667 | 0.328 | 0.306 | 0.588 | 0.573 | 0.611 |
| 2-acetonaphthone | -1.048 | -0.980 | -0.990 | -0.914 | -0.923 | -0.853 |
| 2-chloroaniline | -1.183 | -1.559 | -1.550 | -1.127 | -1.132 | -0.828 |
| 2-heptanone | -0.115 | -0.063 | -0.091 | -0.355 | -0.364 | -0.315 |
| 2-methoxynaphthalene | -0.433 | -0.602 | -0.612 | -0.279 | -0.289 | -0.246 |
| 2-methylbenzothiazole | -0.367 | -0.640 | -0.648 | -0.265 | -0.275 | -0.233 |

| | | | | | | |
|---|--------|--------|--------|--------|--------|--------|
| 1,2,3,4-tetrahydro-6-methylnaphthalene | 0.081 | 0.646 | 0.614 | 0.815 | 0.800 | 0.819 |
| 5,6,7,8-tetrahydro-2-naphthalenol | -2.685 | -1.717 | -1.704 | -1.284 | -1.294 | -1.040 |
| 2-nitrobenzeneamine | -2.242 | -2.382 | -2.365 | -2.446 | -2.449 | -1.982 |
| 2-nitrophenol | -0.935 | -0.969 | -0.972 | -0.999 | -1.005 | -0.926 |
| 2-nitrotoluene | -0.775 | -0.754 | -0.761 | -0.957 | -0.963 | -0.905 |
| benzeneacetamide | -3.013 | -2.634 | -2.624 | -2.215 | -2.217 | -1.845 |
| cyclohexaneethanol | -1.488 | -0.596 | -0.614 | -0.475 | -0.486 | -0.284 |
| 2,4-dimethylaniline | -1.004 | -1.216 | -1.219 | -0.882 | -0.889 | -0.681 |
| 2,4,6,8-tetraethenylcyclohexane | 1.745 | 0.973 | 0.917 | 1.894 | 1.865 | 1.894 |
| 2,5-dichloroaniline | -0.985 | -1.614 | -1.603 | -1.134 | -1.142 | -0.742 |
| 2,6-dimethylcyclohexanol | -1.138 | -0.164 | -0.188 | -0.245 | -0.256 | -0.105 |
| 3-bromophenol | -2.369 | -2.674 | -2.626 | -1.947 | -1.954 | -1.612 |
| 3-methylaniline | -1.137 | -1.615 | -1.609 | -1.190 | -1.195 | -0.930 |
| 3-nitrotoluene | -0.770 | -0.637 | -0.647 | -1.002 | -1.009 | -0.946 |
| 3,4-dichloroaniline | -1.792 | -1.946 | -1.930 | -1.847 | -1.855 | -1.317 |
| 3,5-dimethylphenol | -1.886 | -1.943 | -1.923 | -1.463 | -1.470 | -1.220 |
| 4-acetylbiphenyl | -1.004 | -1.001 | -1.014 | -0.811 | -0.823 | -0.749 |
| 4-bromophenol | -2.670 | -2.757 | -2.709 | -1.895 | -1.901 | -1.572 |
| 4-chlorophenol | -2.233 | -2.628 | -2.582 | -1.899 | -1.905 | -1.576 |
| 3-methyl-4-chlorophenol | -2.071 | -2.307 | -2.271 | -1.737 | -1.745 | -1.427 |
| 4-chloro-2-nitrobenzenamine | -2.321 | -2.397 | -2.381 | -2.442 | -2.447 | -1.904 |
| 4-cyanophenol | -3.268 | -3.861 | -3.793 | -3.120 | -3.123 | -2.654 |
| n,n-dimethyl-4-(phenylazo)-benzeneamine | -1.375 | -0.811 | -0.826 | -1.558 | -1.572 | -1.462 |
| 4-methylbenzaldehyde | -0.703 | -0.763 | -0.774 | -0.875 | -0.882 | -0.823 |
| 4-aminonitrobenzene | -3.821 | -3.682 | -3.648 | -4.434 | -4.435 | -3.486 |
| p-nitrobenzylalcohol | -2.584 | -2.778 | -2.756 | -2.751 | -2.753 | -2.401 |
| 1-methyl-4-nitrobenzene | -0.832 | -0.737 | -0.746 | -1.190 | -1.197 | -1.128 |
| p-hydroxybiphenyl | -2.729 | -2.634 | -2.600 | -1.831 | -1.840 | -1.518 |
| 9,10-dimethylantracene | -0.013 | -0.114 | -0.135 | 0.252 | 0.236 | 0.281 |
| acenaphthylene | -0.229 | -0.422 | -0.432 | -0.042 | -0.053 | -0.014 |
| acetophenone | -0.654 | -0.897 | -0.905 | -0.929 | -0.934 | -0.877 |
| anthraquinone | -0.590 | -1.039 | -1.049 | -0.777 | -0.787 | -0.725 |
| azulene | -0.323 | -0.440 | -0.449 | -0.125 | -0.134 | -0.096 |
| benzamide | -3.075 | -3.075 | -3.053 | -2.712 | -2.712 | -2.230 |
| benz(a)anthracene | -0.414 | -0.602 | -0.614 | -0.028 | -0.045 | 0.018 |
| benzenesulfonamide | -3.984 | -3.896 | -3.862 | -3.830 | -3.828 | -3.319 |
| benzidine | -2.180 | -3.623 | -3.594 | -2.968 | -2.971 | -2.417 |
| benzo[ghi]perylene | -0.618 | -0.567 | -0.581 | 0.011 | -0.007 | 0.061 |
| benzophenone | -0.739 | -0.881 | -0.892 | -0.730 | -0.741 | -0.675 |
| benzo(a)pyrene | -0.615 | -0.585 | -0.598 | -0.024 | -0.042 | 0.024 |
| benzothiazole | -0.768 | -1.051 | -1.051 | -0.508 | -0.515 | -0.462 |
| benzoic acidphenylmethyl ester | -0.602 | -0.843 | -0.858 | -0.387 | -0.401 | -0.341 |
| benzylsalicylate | -0.467 | -0.689 | -0.705 | -0.361 | -0.375 | -0.313 |
| cyclohexylbenzene | -0.067 | 0.647 | 0.614 | 0.903 | 0.887 | 0.909 |
| isoborneol | -0.260 | -0.178 | -0.201 | -0.250 | -0.262 | -0.085 |
| butylbenzylphthalate | -1.022 | -0.982 | -1.011 | -0.885 | -0.905 | -0.805 |
| octadecanoic acidbutylester | 1.863 | 2.888 | 2.778 | 2.907 | 2.862 | 2.904 |
| caffeine | -1.973 | -2.323 | -2.323 | -2.170 | -2.172 | -2.034 |
| camphor | -0.147 | 0.119 | 0.086 | -0.236 | -0.246 | -0.198 |
| carbazole | -2.033 | -1.811 | -1.802 | -1.082 | -1.092 | -0.767 |
| carvon | -0.296 | -0.411 | -0.436 | -0.718 | -0.727 | -0.662 |
| chrysene | -0.452 | -0.665 | -0.676 | -0.088 | -0.104 | -0.039 |
| 2h-1-benzopyran-2-one | -1.637 | -1.549 | -1.549 | -1.807 | -1.811 | -1.719 |
| cyclohexanol | -0.748 | -0.811 | -0.822 | -0.800 | -0.806 | -0.614 |
| dibenzofuran | -0.127 | -0.412 | -0.423 | 0.050 | 0.038 | 0.073 |

| | | | | | | |
|--|--------|--------|--------|--------|--------|--------|
| n-benzyl-1-phenylmethanamine | -0.271 | -0.585 | -0.606 | -0.199 | -0.213 | -0.138 |
| dibenzylether | -0.330 | -0.802 | -0.821 | -0.483 | -0.496 | -0.418 |
| dibutylphthalate | -0.464 | -0.102 | -0.147 | -0.416 | -0.437 | -0.352 |
| adipinsaeurediethylester | -0.595 | -0.756 | -0.790 | -0.810 | -0.819 | -0.749 |
| n,n-diethylcyclohexanamine | 0.121 | 1.463 | 1.414 | 1.355 | 1.336 | 1.358 |
| 1,3-diethyl-1,3-diphenylurea | -0.198 | -0.334 | -0.367 | -0.187 | -0.205 | -0.125 |
| n,n-diethyl-4-nitroaniline | -1.412 | -1.184 | -1.200 | -3.127 | -3.136 | -2.966 |
| diethylphthalate | -1.056 | -0.990 | -1.011 | -1.291 | -1.302 | -1.216 |
| di-2-ethylhexylphthalate | 0.493 | 1.097 | 1.019 | 1.206 | 1.165 | 1.250 |
| diisobutylphthalate | -0.399 | -0.115 | -0.159 | -0.337 | -0.359 | -0.275 |
| n,n-dimethylaniline | -0.128 | -0.279 | -0.295 | -0.203 | -0.212 | -0.173 |
| n,n-dimethyl-4-nitrobenzeneamine | -2.178 | -1.651 | -1.654 | -3.509 | -3.513 | -3.349 |
| dimethylphthalate | -1.480 | -1.477 | -1.484 | -1.642 | -1.648 | -1.564 |
| 1,2-benzenedicarboxylicacid dioctylester | 0.373 | 1.348 | 1.262 | 1.137 | 1.096 | 1.181 |
| n-phenyl-benzeneamine | -1.108 | -1.246 | -1.248 | -0.658 | -0.669 | -0.419 |
| ethylbenzoate | -0.207 | -0.414 | -0.432 | -0.360 | -0.370 | -0.324 |
| eugenol | -1.005 | -0.975 | -0.985 | -0.713 | -0.722 | -0.597 |
| fluoranthene | -0.320 | -0.469 | -0.482 | 0.017 | 0.003 | 0.055 |
| fluorene | -0.059 | -0.344 | -0.358 | 0.080 | 0.068 | 0.107 |
| hexachlorobenzene | 0.583 | 0.947 | 0.912 | 1.165 | 1.146 | 1.163 |
| indole | -2.013 | -2.002 | -1.986 | -1.322 | -1.327 | -0.984 |
| linalool | -0.069 | 0.445 | 0.407 | 0.344 | 0.330 | 0.371 |
| n-methylacetamide | -2.173 | -2.241 | -2.235 | -2.382 | -2.380 | -1.980 |
| methylbenzoate | -0.423 | -0.668 | -0.679 | -0.569 | -0.576 | -0.531 |
| methylnonanoate | 0.548 | 0.575 | 0.530 | 0.580 | 0.561 | 0.600 |
| tetralin | -0.087 | 0.406 | 0.380 | 0.599 | 0.586 | 0.606 |
| niacinamide | -3.369 | -3.749 | -3.719 | -2.886 | -2.884 | -2.368 |
| nitrocyclohexane | -0.842 | -0.189 | -0.209 | -0.631 | -0.638 | -0.591 |
| octanophenon | 0.003 | 0.315 | 0.275 | 0.322 | 0.301 | 0.357 |
| pentachlorophenol | -1.392 | -0.481 | -0.487 | 0.295 | 0.279 | 0.449 |
| perylene | -0.715 | -0.667 | -0.678 | -0.089 | -0.106 | -0.036 |
| phenanthrene | -0.270 | -0.507 | -0.517 | -0.026 | -0.039 | 0.009 |
| cyclohexylbenzene | 0.776 | 0.647 | 0.614 | 0.903 | 0.887 | 0.909 |
| 1,2-benzenedicarbonitrile | -2.569 | -2.256 | -2.243 | -2.739 | -2.743 | -2.604 |
| dl-pin-2(3)-ene | 1.243 | 1.253 | 1.213 | 1.253 | 1.236 | 1.243 |
| beta-pinene | 1.322 | 1.066 | 1.028 | 1.064 | 1.049 | 1.059 |
| benzoicacidphenylester | -0.686 | -0.896 | -0.907 | -0.588 | -0.601 | -0.538 |
| 1,2,3,4-tetrahydroquinoline | -0.643 | -0.720 | -0.731 | -0.581 | -0.590 | -0.424 |
| styrene | 0.134 | 0.298 | -0.308 | 0.024 | 0.016 | 0.044 |
| 1,1'-4',1''-terphenyl | 0.272 | 0.506 | -0.524 | 0.167 | 0.149 | 0.206 |
| 4-methyl-1-(1-methylethyl)-3-cyclohexen-1-ol | 0.023 | -0.453 | 0.418 | 0.307 | 0.293 | 0.376 |
| methylcyclohexane | 0.235 | -1.194 | 1.159 | 1.183 | 1.168 | 1.169 |
| tribenzylamine | 0.349 | -0.061 | 0.026 | 0.844 | 0.820 | 0.874 |
| glycerol-tributyrate | -0.554 | 0.867 | -0.911 | -0.890 | -0.907 | -0.810 |
| triphenylene | -0.582 | 0.721 | -0.731 | -0.160 | -0.176 | -0.106 |
| n-undecane | 1.860 | -2.181 | 2.118 | 2.187 | 2.160 | 2.162 |
| 1-phenyl-1-pentanone | -0.219 | 0.221 | -0.246 | -0.268 | -0.281 | -0.226 |
| 4-hydroxy-3-methoxybenzaldehyde | -2.307 | 1.972 | -1.967 | -1.754 | -1.758 | -1.559 |

Table S7. Experimental and calculated log P for system n-heptane-dimethylsulfoxide at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|--|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-bromohexane | 0.788 | -0.064 | -0.044 | 0.841 | 0.908 | 0.660 |
| 1-bromooctane | 1.176 | 0.151 | 0.174 | 1.395 | 1.483 | 1.151 |
| 1-chloronaphthalene | -0.088 | -0.946 | -0.910 | 0.144 | 0.199 | 0.002 |
| 1-methyl-tetralin | 0.001 | -0.037 | -0.015 | 1.108 | 1.181 | 0.906 |
| 5,6,7,8-tetrahydro-1-naphthalenol | -3.204 | -4.044 | -3.122 | -2.149 | -2.337 | -1.816 |
| 1-nitrohexane | -0.263 | -0.915 | -0.887 | -0.332 | -0.287 | -0.439 |
| 1-nitro-naphthalene | -1.204 | -1.697 | -1.655 | -1.287 | -1.253 | -1.356 |
| a-methylcyclohexanemethanol | -1.997 | -1.267 | -1.129 | -0.733 | -0.708 | -0.767 |
| 1,3-dinitrobenzene | -2.225 | -2.444 | -2.395 | -2.495 | -2.526 | -2.375 |
| 1,2,4,5-tetrachlorobenzene | 0.409 | -0.917 | -0.871 | 0.671 | 0.720 | 0.529 |
| 2-methoxynaphthalene | -0.588 | -1.152 | -1.118 | -0.195 | -0.149 | -0.312 |
| 2-methylbenzothiazole | -0.636 | -1.104 | -1.071 | -0.206 | -0.163 | -0.315 |
| 1,2,3,4-tetrahydro-6-methylnaphthalene | 0.021 | 0.058 | 0.079 | 1.247 | 1.326 | 1.031 |
| 2-methylcyclohexanol | -2.256 | -1.688 | -1.495 | -1.086 | -1.078 | -1.068 |
| 5,6,7,8-tetrahydro-2-naphthalenol | -2.977 | -4.105 | -3.183 | -2.222 | -2.417 | -1.882 |
| 2-nitrobenzeneamine | -2.817 | -3.633 | -3.519 | -3.335 | -3.370 | -3.230 |
| 2-nitropropane | -0.751 | -0.853 | -0.836 | -1.078 | -1.065 | -1.093 |
| 2-nitrotoluene | -0.799 | -1.207 | -1.177 | -1.010 | -0.982 | -1.069 |
| 2-nonanone | 0.328 | -0.166 | -0.147 | 0.642 | 0.716 | 0.446 |
| cyclohexaneethanol | -1.990 | -2.162 | -1.855 | -0.996 | -0.994 | -0.962 |
| 2,4-dimethylaniline | -1.638 | -2.053 | -2.002 | -1.222 | -1.239 | -1.245 |
| 2,4,6,8-tetraethenylcyclotetrasiloxane | 2.263 | -0.060 | -0.023 | 2.669 | 2.806 | 2.280 |
| 2,6-dimethylcyclohexanol | -1.756 | -1.311 | -1.162 | -0.855 | -0.840 | -0.862 |
| 3-hydroxytoluene | -2.525 | -4.576 | -3.560 | -2.788 | -3.017 | -2.369 |
| 3-aminonitrobenzene | -2.992 | -4.069 | -3.962 | -3.611 | -3.673 | -3.515 |
| 3-nitrotoluene | -0.746 | -1.090 | -1.061 | -1.031 | -0.999 | -1.099 |
| 3,4-dichloroaniline | -2.251 | -3.620 | -3.515 | -2.560 | -2.595 | -2.555 |
| 3,5-dimethylphenol | -2.317 | -4.300 | -3.337 | -2.521 | -2.725 | -2.147 |
| 4-bromophenol | -2.953 | -5.528 | -4.268 | -3.031 | -3.302 | -2.579 |
| 3-methyl-4-chlorophenol | -2.444 | -5.047 | -3.861 | -2.781 | -3.050 | -2.349 |
| 4-chloro-2-nitrobenzenamine | -2.602 | -4.067 | -3.926 | -3.416 | -3.466 | -3.279 |
| p-fluoroaniline | -1.928 | -3.081 | -3.008 | -2.091 | -2.146 | -2.042 |
| 4-methylaniline | -1.846 | -2.472 | -2.413 | -1.560 | -1.584 | -1.565 |
| 4-methylbenzaldehyde | -0.849 | -1.118 | -1.092 | -0.733 | -0.699 | -0.807 |
| 4-aminonitrobenzene | -3.800 | -5.562 | -5.374 | -5.844 | -5.946 | -5.570 |
| 1-methyl-4-nitrobenzene | -0.787 | -1.181 | -1.152 | -1.235 | -1.205 | -1.294 |
| p-hydroxybiphenyl | -3.191 | -5.342 | -4.216 | -2.917 | -3.168 | -2.510 |
| 8-quinolinol | -1.435 | -1.872 | -1.806 | -0.840 | -0.800 | -0.933 |
| 9,10-dimethylanthracene | -0.234 | -0.873 | -0.835 | 0.450 | 0.523 | 0.255 |
| acenaphthylene | -0.407 | -1.030 | -0.995 | -0.015 | 0.034 | -0.141 |
| acetanilide | -3.076 | -3.256 | -3.147 | -3.109 | -3.173 | -2.910 |
| acetophenone | -0.827 | -1.249 | -1.221 | -0.864 | -0.837 | -0.921 |
| cyclohexylamine | -1.646 | -0.491 | -0.473 | 0.084 | 0.111 | 0.017 |
| anisole | -0.318 | -0.882 | -0.858 | -0.235 | -0.203 | -0.312 |
| anthraquinone | -1.016 | -1.759 | -1.714 | -0.673 | -0.625 | -0.786 |
| azulene | -0.587 | -0.954 | -0.924 | -0.095 | -0.053 | -0.201 |
| benzaldehyde | -0.898 | -1.340 | -1.311 | -0.932 | -0.910 | -0.974 |
| benzamide | -3.918 | -4.476 | -4.340 | -4.300 | -4.310 | -4.191 |

| | | | | | | |
|--|--------|--------|--------|--------|--------|--------|
| benz(a)anthracene | -0.664 | -1.519 | -1.468 | -0.004 | 0.064 | -0.181 |
| benzo[ghi]perylene | -1.558 | -1.634 | -1.578 | 0.029 | 0.106 | -0.170 |
| benzophenone | -0.778 | -1.496 | -1.456 | -0.625 | -0.574 | -0.749 |
| benzonitrile | -0.974 | -1.665 | -1.631 | -1.295 | -1.274 | -1.329 |
| benzo(a)pyrene | -1.052 | -1.580 | -1.526 | -0.009 | 0.064 | -0.195 |
| benzo(e)pyrene | -1.231 | -1.670 | -1.615 | -0.115 | -0.046 | -0.291 |
| benzothiazole | -1.234 | -1.728 | -1.685 | -0.617 | -0.596 | -0.664 |
| cyclohexanemethanol | -2.186 | -2.123 | -1.839 | -1.022 | -1.013 | -1.005 |
| benzoicacidphenylmethylester | -0.665 | -1.556 | -1.512 | -0.237 | -0.173 | -0.400 |
| cyclohexylbenzene | -0.175 | -0.013 | 0.012 | 1.341 | 1.426 | 1.107 |
| benzoicacidbutylester | 0.232 | -0.602 | -0.572 | 0.491 | 0.565 | 0.296 |
| butylbenzylphthalate | -1.111 | -1.884 | -1.829 | -0.446 | -0.348 | -0.695 |
| octadecanoicacidbutylester | 2.504 | 1.412 | 1.446 | 4.567 | 4.776 | 3.976 |
| caffeine | -2.550 | -2.788 | -2.740 | -2.297 | -2.336 | -2.184 |
| carbazole | -2.660 | -3.210 | -3.078 | -2.102 | -2.106 | -2.059 |
| chrysene | -0.877 | -1.616 | -1.564 | -0.117 | -0.052 | -0.282 |
| 2h-1-benzopyran-2-one | -1.935 | -2.099 | -2.059 | -1.930 | -1.914 | -1.935 |
| dibenzofuran | -0.352 | -1.136 | -1.097 | 0.052 | 0.105 | -0.083 |
| n-benzyl-1-phenylmethanamine | -0.574 | -1.225 | -1.186 | -0.109 | -0.052 | -0.259 |
| dibenzylether | -0.437 | -1.368 | -1.329 | -0.287 | -0.228 | -0.434 |
| dibutylphthalate | -0.118 | -0.902 | -0.863 | 0.341 | 0.448 | 0.059 |
| adipinsaeurediethylester | -0.441 | -1.046 | -1.021 | -0.298 | -0.240 | -0.439 |
| 1,3-diethyl-1,3-diphenylurea | -0.829 | -1.043 | -1.004 | 0.230 | 0.318 | 0.000 |
| n,n-diethyl-4-nitroaniline | -1.483 | -1.628 | -1.592 | -3.129 | -3.087 | -3.187 |
| diethylphthalate | -1.097 | -1.515 | -1.478 | -0.987 | -0.928 | -1.122 |
| di-2-ethylhexylphthalate | 0.707 | -0.194 | -0.146 | 2.626 | 2.807 | 2.126 |
| diisobutylphthalate | -0.261 | -0.900 | -0.861 | 0.398 | 0.506 | 0.114 |
| n,n-dimethylaniline | -0.064 | -0.656 | -0.633 | -0.047 | -0.004 | -0.157 |
| n,n-dimethyl-4-nitrobenzeneamine | -1.978 | -1.997 | -1.960 | -3.688 | -3.669 | -3.679 |
| dimethylphthalate | -1.557 | -1.932 | -1.893 | -1.625 | -1.595 | -1.678 |
| 1,2-benzenedicarboxylicacid dioctylester | 0.810 | -0.040 | 0.010 | 2.576 | 2.764 | 2.058 |
| diphenylether | -0.179 | -1.096 | -1.058 | 0.142 | 0.199 | -0.006 |
| dodecane | 2.707 | 1.283 | 1.304 | 3.310 | 3.457 | 2.894 |
| ethylbenzoate | -0.173 | -0.895 | -0.867 | -0.141 | -0.092 | -0.265 |
| fluoranthene | -0.683 | -1.258 | -1.214 | 0.076 | 0.140 | -0.090 |
| fluorene | -0.244 | -0.948 | -0.914 | 0.200 | 0.256 | 0.053 |
| hexachlorobenzene | 0.333 | -0.196 | -0.157 | 1.595 | 1.689 | 1.333 |
| indole | -2.594 | -3.292 | -3.155 | -2.316 | -2.333 | -2.239 |
| iodobenzene | -0.128 | -0.960 | -0.926 | -0.016 | 0.027 | -0.127 |
| methylbenzoate | -0.398 | -1.117 | -1.087 | -0.485 | -0.449 | -0.570 |
| decanoicacidmethylester | 1.061 | 0.072 | 0.095 | 1.548 | 1.650 | 1.270 |
| methyloctanoate | 0.653 | -0.149 | -0.129 | 0.972 | 1.051 | 0.759 |
| tetralin | -0.182 | -0.112 | -0.092 | 0.932 | 0.998 | 0.752 |
| nitrocyclohexane | -1.017 | -0.462 | -0.446 | -0.384 | -0.345 | -0.475 |
| octadecane | 3.280 | 1.927 | 1.956 | 4.824 | 5.031 | 4.236 |
| 1-octanol | -0.643 | -2.004 | -1.693 | -0.600 | -0.583 | -0.608 |
| octanophenon | 0.388 | -0.469 | -0.436 | 0.901 | 0.996 | 0.645 |
| pentachlorophenol | -2.035 | -2.898 | -2.174 | -0.249 | -0.225 | -0.317 |
| perylene | -1.118 | -1.688 | -1.632 | -0.120 | -0.051 | -0.295 |
| phenanthrene | -0.508 | -1.237 | -1.196 | -0.003 | 0.053 | -0.146 |
| phthalimide | -3.059 | -3.992 | -3.816 | -3.715 | -3.776 | -3.465 |
| 1,2-benzenedicarbonitrile | -2.461 | -2.892 | -2.838 | -3.234 | -3.251 | -3.129 |
| phenylacetate | -0.959 | -1.534 | -1.502 | -0.969 | -0.944 | -1.019 |
| benzoicacidphenylester | -0.798 | -1.632 | -1.587 | -0.553 | -0.499 | -0.689 |
| pyrene | -0.570 | -1.220 | -1.177 | 0.106 | 0.169 | -0.058 |
| 1,1'-4',1''-terphenyl | 0.076 | -1.397 | -1.348 | 0.259 | 0.336 | 0.058 |
| tetradecane | 3.020 | 1.499 | 1.522 | 3.836 | 4.004 | 3.359 |
| glycerol-tributyrate | -0.442 | -1.554 | -1.513 | -0.256 | -0.162 | -0.491 |
| triphenylene | -1.024 | -1.715 | -1.661 | -0.244 | -0.183 | -0.396 |

| | | | | | | |
|--------------------------|--------|--------|--------|-------|-------|--------|
| n,n-diphenylbenzeneamine | 0.345 | -1.117 | -1.070 | 0.717 | 0.803 | 0.487 |
| n-undecane | 2.165 | 1.178 | 1.198 | 3.049 | 3.185 | 2.662 |
| 1-phenyl-1-pentanone | -0.163 | -0.791 | -0.761 | 0.051 | 0.114 | -0.108 |

Table S8. Exp. and calculated log P for system n-heptane- formamide at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|----------------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-Acetonaphthone | 0.131 | 0.563 | 0.558 | 0.629 | 0.658 | 0.607 |
| 1-Bromododecane | 3.540 | 4.997 | 4.983 | 3.874 | 3.879 | 3.888 |
| 1-Bromonaphthalene | 1.370 | 1.452 | 1.448 | 1.751 | 1.754 | 1.759 |
| 1-Bromooctane | 2.566 | 3.289 | 3.279 | 2.452 | 2.455 | 2.462 |
| 1-Chloronaphthalene | 1.377 | 1.532 | 1.527 | 1.745 | 1.748 | 1.753 |
| 1-Hydroxyanthraquinone | 0.361 | 0.506 | 0.501 | 1.071 | 1.081 | 1.077 |
| 1-Methylnaphthalene | 1.406 | 2.489 | 2.481 | 2.305 | 2.308 | 2.314 |
| 1-Naphthol | -1.967 | -0.858 | -0.830 | -0.748 | -0.701 | -0.739 |
| 1-Nitronaphthalene | 0.094 | 0.280 | 0.277 | 0.472 | 0.481 | 0.476 |
| 1-Phenylethanol | -1.190 | 0.872 | 0.867 | -0.052 | -0.046 | -0.075 |
| 1,3-Dinitrobenzene | -1.427 | -0.966 | -0.968 | -0.819 | -0.812 | -0.816 |
| 1,4-Dichlorobenzene | 1.242 | 1.230 | 1.226 | 1.316 | 1.318 | 1.322 |
| 1,2,4,5-Tetrachlorobenzene | 1.897 | 2.093 | 2.088 | 1.828 | 1.832 | 1.836 |
| 2-Acetonaphthone | -0.027 | 0.427 | 0.422 | 0.546 | 0.584 | 0.518 |
| 2-Chloroaniline | -0.467 | -0.424 | -0.425 | -0.310 | -0.263 | -0.339 |
| 2-Chlorophenol | -1.145 | -0.365 | -0.361 | 0.450 | 0.452 | 0.462 |
| 2-Methoxynaphthalene | 0.796 | 1.125 | 1.120 | 1.408 | 1.411 | 1.415 |
| 2-Methylaniline | -1.130 | -0.367 | -0.369 | -0.421 | -0.394 | -0.430 |
| 2-Methylnaphthalene | 1.366 | 2.667 | 2.659 | 2.448 | 2.451 | 2.457 |
| 2-Methylphenol | -1.662 | 0.352 | 0.350 | -0.493 | -0.484 | -0.519 |
| 2-Naphthol | -2.257 | -0.999 | -0.971 | -0.890 | -0.838 | -0.880 |
| 2-Nitroaniline | -1.793 | -1.792 | -1.792 | -1.872 | -1.746 | -1.996 |
| 2-Nitrophenol | -0.496 | -0.258 | -0.261 | 0.177 | 0.179 | 0.182 |
| 2-Nitrotoluene | 0.097 | 0.346 | 0.343 | 0.291 | 0.300 | 0.294 |
| 2-Nonanone | 0.947 | 2.074 | 2.065 | 1.199 | 1.235 | 1.160 |
| 2-Octanone | 0.769 | 1.632 | 1.625 | 0.858 | 0.894 | 0.819 |
| 2,4-Dichlorophenol | -1.135 | -0.231 | -0.224 | 0.544 | 0.557 | 0.546 |
| 3-Bromophenol | -2.368 | -2.468 | -2.406 | -1.920 | -1.812 | -1.936 |
| 3-Methylaniline | -0.733 | -0.502 | -0.504 | -0.454 | -0.425 | -0.465 |
| 3-Nitroaniline | -2.513 | -1.974 | -1.973 | -2.103 | -1.965 | -2.212 |
| 3-Nitrotoluene | 0.262 | 0.487 | 0.483 | 0.302 | 0.311 | 0.305 |
| 3,4-Dichloroaniline | -1.009 | -0.721 | -0.722 | -1.028 | -0.921 | -1.107 |
| 4-Acetylbiphenyl | 0.295 | 0.703 | 0.697 | 0.938 | 0.979 | 0.908 |
| 4-Chloroaniline | -0.983 | -0.894 | -0.895 | -0.942 | -0.874 | -0.983 |
| 4-Chloro-3-methylphenol | -1.916 | -1.959 | -1.909 | -1.611 | -1.517 | -1.621 |
| 4-Chloro-2-nitroaniline | -1.861 | -1.643 | -1.643 | -1.826 | -1.695 | -1.970 |
| 4-Cyanophenol | -3.204 | -4.195 | -4.104 | -3.291 | -3.096 | -3.349 |
| 4-Dimethylaminoazobenzene | -0.635 | 1.774 | 1.767 | 0.697 | 0.730 | 0.685 |
| 4-Fluoroaniline | -1.223 | -1.088 | -1.089 | -0.941 | -0.897 | -0.961 |
| 4-Methylaniline | -0.722 | -0.473 | -0.475 | -0.394 | -0.369 | -0.402 |
| 4-Methylbenzaldehyde | -0.087 | 0.226 | 0.222 | 0.200 | 0.240 | 0.174 |
| 4-Nitrobenzyl alcohol | -2.363 | -2.706 | -2.692 | -2.488 | -2.429 | -2.539 |
| 4-Nitrotoluene | -0.014 | 0.354 | 0.351 | 0.093 | 0.106 | 0.094 |
| 4-Phenylphenol | -2.103 | -1.901 | -1.857 | -1.109 | -1.027 | -1.111 |
| 8-Hydroxyquinoline | -0.618 | 0.278 | 0.275 | 0.713 | 0.706 | 0.728 |
| Acenaphthylene | 0.894 | 1.300 | 1.295 | 1.715 | 1.718 | 1.723 |
| Acetophenone | -0.255 | 0.050 | 0.046 | 0.052 | 0.086 | 0.023 |
| Aniline | -1.029 | 0.713 | 0.713 | -0.604 | -0.612 | -0.537 |
| Anise Alcohol | -2.074 | -1.378 | -1.376 | -1.356 | -1.325 | -1.388 |

| | | | | | | |
|-----------------------------|--------|--------|--------|--------|--------|--------|
| Azulene | 0.757 | 1.135 | 1.130 | 1.430 | 1.433 | 1.437 |
| Benzaldehyde | -0.275 | -0.190 | -0.192 | 0.010 | 0.038 | -0.006 |
| Benz[a]anthracene | 1.425 | 1.823 | 1.817 | 2.467 | 2.472 | 2.479 |
| Benzidine | -1.555 | -2.189 | -2.190 | -2.085 | -2.019 | -2.118 |
| Benzo[ghi]perylene | 1.563 | 2.044 | 2.037 | 2.750 | 2.755 | 2.763 |
| Benzophenone | 0.393 | 0.675 | 0.670 | 0.931 | 0.974 | 0.905 |
| Benzonitrile | -0.376 | -0.236 | -0.238 | -0.032 | -0.016 | -0.033 |
| Benzothiazole | -0.423 | 0.064 | 0.062 | 0.382 | 0.385 | 0.372 |
| Benzyl alcohol | -1.767 | 0.046 | 0.045 | -0.270 | -0.248 | -0.305 |
| Benzyl benzoate | 0.843 | 1.133 | 1.127 | 1.658 | 1.675 | 1.661 |
| Benzyl salicylate | 1.117 | 1.319 | 1.313 | 1.827 | 1.834 | 1.836 |
| Biphenyl | 1.309 | 2.833 | 2.824 | 2.683 | 2.686 | 2.693 |
| Borneol | 0.273 | 0.989 | 0.985 | 0.028 | 0.050 | 0.000 |
| Butyl benzyl phthalate | 1.059 | 1.762 | 1.752 | 1.638 | 1.681 | 1.629 |
| Caffeine | -1.876 | -1.726 | -1.729 | -1.844 | -1.832 | -1.865 |
| Camphor | 0.460 | 1.433 | 1.426 | 0.635 | 0.681 | 0.589 |
| Carbazole | -0.716 | -0.268 | -0.270 | 0.167 | 0.212 | 0.118 |
| Chlorobenzene | 1.097 | 1.048 | 1.045 | 1.148 | 1.151 | 1.154 |
| Chrysene | 1.657 | 1.703 | 1.697 | 2.380 | 2.385 | 2.391 |
| Coumarin | -1.314 | -0.846 | -0.848 | -0.755 | -0.688 | -0.800 |
| Decan-1-ol | 0.928 | 1.709 | 1.705 | 0.820 | 0.854 | 0.782 |
| Dibenzofuran | 1.206 | 1.324 | 1.320 | 1.908 | 1.911 | 1.916 |
| Dibenzylamine | 0.709 | 1.671 | 1.664 | 1.324 | 1.316 | 1.348 |
| Dibenzyl ether | 1.078 | 1.296 | 1.289 | 1.436 | 1.464 | 1.413 |
| Dibutyl phthalate | 1.373 | 2.572 | 2.561 | 1.752 | 1.798 | 1.741 |
| Diethyl adipate | 0.272 | 0.844 | 0.836 | 0.333 | 0.370 | 0.311 |
| Diethyl phthalate | -0.010 | 0.663 | 0.656 | 0.253 | 0.298 | 0.237 |
| Di-2-ethylhexyl phthalate | 3.368 | 5.233 | 5.215 | 4.286 | 4.338 | 4.279 |
| Diisobutyl phthalate | 1.350 | 2.473 | 2.462 | 1.755 | 1.803 | 1.743 |
| N,N-Dimethylaniline | 0.766 | 1.316 | 1.310 | 1.156 | 1.159 | 1.162 |
| N,N-Dimethyl-4-nitroaniline | -1.060 | -0.616 | -0.620 | -2.103 | -1.987 | -2.201 |
| Dimethyl phthalate | -0.743 | -0.303 | -0.307 | -0.366 | -0.333 | -0.377 |
| Dioctyl phthalate | 3.465 | 6.000 | 5.980 | 4.367 | 4.417 | 4.361 |
| Diphenylamine | 0.188 | 0.590 | 0.586 | 0.988 | 1.023 | 0.960 |
| Diphenyl ether | 1.375 | 1.489 | 1.483 | 2.036 | 2.039 | 2.045 |
| Ethyl benzoate | 0.606 | 0.947 | 0.942 | 1.006 | 1.026 | 1.002 |
| Eugenol | -0.456 | 0.382 | 0.379 | 0.563 | 0.565 | 0.579 |
| Fluoranthene | 1.424 | 1.699 | 1.693 | 2.238 | 2.243 | 2.248 |
| Fluorene | 1.388 | 1.589 | 1.583 | 1.977 | 1.980 | 1.985 |
| Hexachlorobenzene | 2.237 | 3.069 | 3.061 | 2.454 | 2.457 | 2.463 |
| Indole | -1.354 | -0.977 | -0.978 | -0.563 | -0.512 | -0.626 |
| Iodobenzene | 0.947 | 1.072 | 1.068 | 1.227 | 1.230 | 1.233 |
| Limonene | 2.295 | 2.944 | 2.935 | 2.504 | 2.507 | 2.513 |
| Linalool | 0.610 | 2.131 | 2.122 | 1.215 | 1.215 | 1.191 |
| Methyl benzoate | 0.298 | 0.466 | 0.462 | 0.627 | 0.644 | 0.625 |
| Methyl nonanoate | 1.810 | 2.749 | 2.739 | 2.110 | 2.135 | 2.104 |
| Naphthalene | 1.198 | 2.185 | 2.178 | 2.079 | 2.082 | 2.087 |
| Nitrobenzene | -0.301 | 1.010 | 1.005 | 0.403 | 0.411 | 0.406 |
| Nonan-1-ol | 0.734 | 1.294 | 1.291 | 0.509 | 0.542 | 0.470 |
| Octanal | 1.030 | 1.810 | 1.803 | 1.221 | 1.247 | 1.206 |
| Octan-1-ol | 0.266 | 0.868 | 0.866 | 0.208 | 0.241 | 0.168 |
| Perylene | 1.331 | 1.793 | 1.787 | 2.505 | 2.511 | 2.517 |
| Phenanthrene | 1.252 | 1.461 | 1.455 | 1.993 | 1.997 | 2.002 |
| Phenol | -2.304 | -0.386 | -0.386 | -0.969 | -0.951 | -1.006 |
| Phenylcyclohexane | 2.159 | 2.833 | 2.824 | 2.683 | 2.686 | 2.693 |
| Phthalimide | -2.387 | -2.423 | -2.422 | -2.129 | -2.108 | -2.107 |
| Phthalonitrile | -1.973 | -1.151 | -1.152 | -1.518 | -1.504 | -1.518 |
| alpha-Pinene | 2.426 | 3.268 | 3.260 | 2.697 | 2.700 | 2.707 |
| beta-Pinene | 2.256 | 3.039 | 3.031 | 2.444 | 2.447 | 2.453 |
| Phenyl acetate | -0.214 | -0.079 | -0.083 | 0.223 | 0.241 | 0.220 |
| Phenyl benzoate | 0.635 | 0.860 | 0.855 | 1.345 | 1.362 | 1.349 |
| Phenylcyclohexane | 2.159 | 2.833 | 2.824 | 2.683 | 2.686 | 2.693 |
| Quinoline | -0.235 | 0.788 | 0.783 | 0.552 | 0.572 | 0.550 |
| Styrene | 1.126 | 1.131 | 1.127 | 1.410 | 1.413 | 1.417 |
| Terpinen-4-ol | 0.845 | 2.067 | 2.059 | 1.061 | 1.058 | 1.055 |

| | | | | | | |
|------------------------|--------|--------|--------|--------|--------|--------|
| Tribenzylamine | 2.877 | 3.324 | 3.313 | 3.930 | 3.936 | 3.945 |
| Tri- <i>n</i> -butyrin | 1.004 | 1.641 | 1.629 | 1.050 | 1.080 | 1.043 |
| Triphenylene | 1.263 | 1.594 | 1.588 | 2.284 | 2.289 | 2.294 |
| Triphenylamine | 2.719 | 2.492 | 2.484 | 3.255 | 3.259 | 3.268 |
| Triphenylmethane | 2.495 | 6.104 | 6.089 | 5.196 | 5.200 | 5.212 |
| Valerophenone | 0.863 | 1.521 | 1.514 | 1.253 | 1.288 | 1.233 |
| Vanillin | -2.044 | -1.634 | -1.629 | -1.178 | -1.102 | -1.239 |

Table S9. Experimental and calculated log P for system n-heptane- ethylene glycol at 25 °C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|----------------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-Acetonaphthone | 0.413 | -0.168 | -0.151 | 0.000 | 0.000 | -0.141 |
| 1-Bromododecane | 3.498 | 2.366 | 2.310 | 2.822 | 2.822 | 2.849 |
| 1-Chloronaphthalene | 1.351 | 0.583 | 0.568 | 0.912 | 0.912 | 0.916 |
| 1-Hydroxyanthraquinone | 0.475 | 0.062 | 0.060 | 0.259 | 0.259 | 0.207 |
| 1-Iodobutane | 1.498 | 0.702 | 0.683 | 0.800 | 0.800 | 0.804 |
| 1-Methylnaphthalene | 1.353 | 1.147 | 1.118 | 1.460 | 1.460 | 1.472 |
| 1-Naphthol | -2.193 | -1.612 | -1.227 | -1.026 | -1.026 | -1.367 |
| 1-Nitronaphthalene | 0.448 | -0.106 | -0.107 | -0.191 | -0.191 | -0.239 |
| 1-Phenylethanol | -1.191 | -0.481 | -0.337 | -0.206 | -0.206 | -0.405 |
| 1,2-Dichlorobenzene | 1.364 | 0.491 | 0.478 | 0.671 | 0.671 | 0.673 |
| 1,2-Dimethylbenzene | 1.370 | 1.561 | 1.526 | 1.832 | 1.832 | 1.855 |
| 1,3-Dinitrobenzene | -0.582 | -0.722 | -0.711 | -1.125 | -1.125 | -1.188 |
| 1,4-Dimethylbenzene | 1.460 | 0.799 | 0.778 | 1.044 | 1.044 | 1.052 |
| 1,2,4,5-Tetrachlorobenzene | 1.814 | 0.924 | 0.903 | 1.362 | 1.362 | 1.367 |
| 2-Acetonaphthone | 0.255 | -0.293 | -0.268 | 0.001 | 0.001 | -0.165 |
| 2-Chloroaniline | -0.462 | -0.968 | -0.940 | -0.713 | -0.713 | -0.876 |
| 2-Heptanone | 0.889 | 0.095 | 0.131 | 0.323 | 0.323 | 0.160 |
| 2-Methoxynaphthalene | 0.945 | 0.293 | 0.283 | 0.559 | 0.559 | 0.549 |
| 2-Methylaniline | -0.614 | -0.941 | -0.907 | -0.806 | -0.806 | -0.959 |
| 2-Methylbenzothiazole | 0.368 | -0.061 | -0.023 | 0.250 | 0.250 | 0.144 |
| 2-Methylnaphthalene | 1.337 | 1.249 | 1.217 | 1.570 | 1.570 | 1.584 |
| 2-Methylphenol | -1.499 | -0.792 | -0.636 | -0.538 | -0.538 | -0.771 |
| 2-Naphthol | -2.464 | -1.733 | -1.341 | -1.139 | -1.139 | -1.510 |
| 2-Nitroaniline | -1.413 | -1.812 | -1.753 | -1.886 | -1.886 | -2.403 |
| 2-Nitrophenol | 0.032 | -0.294 | -0.289 | -0.269 | -0.269 | -0.280 |
| 2-Nitropropane | -0.015 | -0.143 | -0.144 | -0.501 | -0.501 | -0.539 |
| 2-Nitrotoluene | 0.452 | -0.011 | -0.014 | -0.160 | -0.160 | -0.203 |
| 2-Nonanone | 1.657 | 0.539 | 0.563 | 0.823 | 0.823 | 0.656 |
| 2-Phenylacetamide | -2.656 | -2.864 | -2.608 | -1.889 | -1.889 | -2.543 |
| 2-Phenylethanol | -1.114 | -1.049 | -0.837 | -0.554 | -0.554 | -0.846 |
| 2,5-Dichloroaniline | -0.416 | -0.996 | -0.967 | -0.681 | -0.681 | -0.925 |
| 2,6-Dimethylphenol | -0.684 | -0.440 | -0.310 | -0.270 | -0.270 | -0.470 |
| 3-Bromophenol | -2.595 | -2.662 | -2.068 | -1.746 | -1.746 | -2.373 |
| 3-Methylaniline | -0.717 | -1.093 | -1.047 | -0.890 | -0.890 | -1.052 |
| 3-Methylphenol | -2.075 | -2.284 | -1.833 | -1.635 | -1.635 | -2.042 |
| 3-Nitrotoluene | 0.471 | 0.101 | 0.095 | -0.174 | -0.174 | -0.220 |
| 3,4-Dichloroaniline | -1.226 | -1.334 | -1.294 | -1.292 | -1.292 | -1.684 |
| 3,5-Dimethylphenol | -1.463 | -1.968 | -1.550 | -1.382 | -1.382 | -1.740 |
| 4-Acetylbiphenyl | 0.688 | -0.177 | -0.153 | 0.210 | 0.210 | 0.032 |
| 4-Bromophenol | -2.222 | -2.731 | -2.155 | -1.724 | -1.724 | -2.287 |
| 4-Chloroaniline | -1.281 | -1.386 | -1.342 | -1.242 | -1.242 | -1.523 |
| 4-Chlorophenol | -2.469 | -2.728 | -2.153 | -1.762 | -1.762 | -2.327 |
| 4-Chloro-3-methylphenol | -2.023 | -2.371 | -1.837 | -1.546 | -1.546 | -2.116 |
| 4-Chloro-2-nitroaniline | -1.274 | -1.789 | -1.728 | -1.853 | -1.853 | -2.435 |
| 4-Cyanophenol | -3.249 | -4.078 | -3.289 | -2.840 | -2.840 | -3.820 |

| | | | | | | |
|-----------------------------|--------|--------|--------|--------|--------|--------|
| 4-Dimethylaminoazobenzene | -0.549 | 0.362 | 0.353 | -0.129 | -0.129 | -0.255 |
| 4-Fluoroaniline | -1.167 | -1.506 | -1.450 | -1.280 | -1.280 | -1.509 |
| 4-Methylaniline | -0.776 | -1.097 | -1.041 | -0.849 | -0.849 | -1.007 |
| 4-Methylbenzaldehyde | 0.311 | -0.304 | -0.282 | -0.165 | -0.165 | -0.327 |
| 4-Methylphenol | -1.862 | -2.272 | -1.835 | -1.613 | -1.613 | -1.999 |
| 4-Nitroaniline | -3.000 | -3.227 | -3.115 | -3.720 | -3.720 | -5.048 |
| 4-Nitrobenzyl alcohol | -2.133 | -2.644 | -2.347 | -2.518 | -2.518 | -2.969 |
| 4-Nitrotoluene | 0.461 | 0.002 | -0.001 | -0.328 | -0.328 | -0.388 |
| 4-Phenylphenol | -2.172 | -2.364 | -1.869 | -1.457 | -1.457 | -1.972 |
| 8-Hydroxyquinoline | -0.360 | -0.279 | -0.268 | 0.023 | 0.023 | 0.056 |
| Acenaphthylene | 1.180 | 0.433 | 0.420 | 0.759 | 0.759 | 0.758 |
| Acetanilide | -2.108 | -1.927 | -1.804 | -1.684 | -1.684 | -2.270 |
| Acetophenone | 0.390 | -0.441 | -0.412 | -0.246 | -0.246 | -0.401 |
| Anise Alcohol | -1.929 | -1.892 | -1.702 | -1.603 | -1.603 | -1.842 |
| Anthraquinone | 0.713 | -0.154 | -0.149 | 0.150 | 0.150 | 0.076 |
| Azulene | 0.693 | 0.344 | 0.332 | 0.610 | 0.610 | 0.607 |
| Benzaldehyde | 0.124 | -0.508 | -0.486 | -0.337 | -0.337 | -0.460 |
| Benzamide | -2.972 | -3.214 | -3.007 | -2.478 | -2.478 | -3.290 |
| Benzenesulfonamide | -3.661 | -3.356 | -3.242 | -4.020 | -4.020 | -4.321 |
| Benzidine | -1.198 | -2.721 | -2.628 | -2.719 | -2.719 | -3.049 |
| Benzophenone | 0.909 | -0.083 | -0.071 | 0.287 | 0.287 | 0.124 |
| Benzonitrile | 0.007 | -0.634 | -0.617 | -0.518 | -0.518 | -0.599 |
| Benzo[a]pyrene | 1.336 | 0.681 | 0.662 | 1.173 | 1.173 | 1.170 |
| Benzothiazole | -0.138 | -0.551 | -0.501 | -0.089 | -0.089 | -0.197 |
| Benzyl alcohol | -1.600 | -1.064 | -0.877 | -0.471 | -0.471 | -0.692 |
| Benzyl benzoate | 1.134 | 0.192 | 0.191 | 0.711 | 0.711 | 0.638 |
| Benzyl salicylate | 1.466 | 0.435 | 0.423 | 0.713 | 0.713 | 0.684 |
| Biphenyl | 1.468 | 1.302 | 1.270 | 1.719 | 1.719 | 1.733 |
| Borneol | 0.511 | -0.387 | -0.260 | -0.222 | -0.222 | -0.445 |
| Bromobenzene | 0.970 | 0.786 | 0.765 | 0.789 | 0.789 | 0.791 |
| Butyl benzoate | 1.596 | 0.688 | 0.680 | 0.998 | 0.998 | 0.911 |
| Butyl benzyl phthalate | 1.420 | 0.314 | 0.315 | 0.682 | 0.682 | 0.494 |
| Caffeine | -1.345 | -2.138 | -2.027 | -1.636 | -1.636 | -1.847 |
| Camphor | 0.868 | 0.296 | 0.318 | 0.450 | 0.450 | 0.259 |
| Carvone | 0.731 | -0.132 | -0.080 | 0.084 | 0.084 | -0.155 |
| Chrysene | 1.449 | 0.546 | 0.530 | 1.048 | 1.048 | 1.043 |
| Coumarin | -0.848 | -1.043 | -0.998 | -0.975 | -0.975 | -1.250 |
| Cyclohexanone | 0.094 | -0.423 | -0.371 | -0.248 | -0.248 | -0.447 |
| Dibenzylamine | 0.673 | 0.162 | 0.267 | 0.807 | 0.807 | 0.762 |
| Dibenzyl ether | 1.202 | 0.093 | 0.119 | 0.680 | 0.680 | 0.572 |
| Dibutyl phthalate | 1.741 | 0.863 | 0.852 | 0.995 | 0.995 | 0.802 |
| Diethyl adipate | 0.942 | -0.222 | -0.190 | 0.137 | 0.137 | -0.052 |
| N,N-Diethylaniline | 1.458 | 1.409 | 1.726 | 2.111 | 2.111 | 2.149 |
| N,N-Diethyl-4-nitroaniline | 0.110 | -0.432 | -0.407 | -1.512 | -1.512 | -1.963 |
| Diethyl phthalate | 0.512 | -0.145 | -0.134 | -0.162 | -0.162 | -0.364 |
| Di-2-ethylhexyl phthalate | 3.612 | 2.196 | 2.159 | 3.015 | 3.015 | 2.817 |
| Diisobutyl phthalate | 1.776 | 0.815 | 0.805 | 0.964 | 0.964 | 0.757 |
| N,N-Dimethylaniline | 0.983 | 0.442 | 0.427 | 0.512 | 0.512 | 0.504 |
| N,N-Dimethyl-4-nitroaniline | -0.388 | -0.927 | -0.892 | -2.045 | -2.045 | -2.469 |
| Dimethyl phthalate | -0.254 | -0.650 | -0.630 | -0.626 | -0.626 | -0.789 |
| Diethyl phthalate | 3.794 | 2.575 | 2.528 | 3.015 | 3.015 | 2.815 |
| Diphenylamine | 0.209 | -0.267 | -0.260 | 0.038 | 0.038 | -0.082 |
| Diphenyl ether | 1.369 | 0.557 | 0.541 | 0.984 | 0.984 | 0.984 |
| Ethylbenzene | 1.400 | 0.762 | 0.741 | 1.019 | 1.019 | 1.026 |
| Ethyl benzoate | 0.813 | 0.176 | 0.179 | 0.449 | 0.449 | 0.365 |
| Eugenol | -0.270 | -0.368 | -0.314 | -0.177 | -0.177 | -0.189 |
| Fluoranthene | 1.141 | 0.607 | 0.589 | 1.022 | 1.022 | 1.021 |
| Fluorene | 1.261 | 0.581 | 0.563 | 0.965 | 0.965 | 0.966 |
| Hexachlorobenzene | 2.098 | 1.604 | 1.567 | 2.040 | 2.040 | 2.061 |
| Indole | -1.254 | -1.332 | -1.284 | -1.083 | -1.083 | -1.321 |
| Iodobenzene | 1.028 | 0.361 | 0.351 | 0.684 | 0.684 | 0.687 |
| Limonene | 2.202 | 1.407 | 1.373 | 1.670 | 1.670 | 1.683 |

| | | | | | | |
|-------------------|--------|--------|--------|--------|--------|--------|
| Methyl benzoate | 0.586 | -0.061 | -0.055 | 0.153 | 0.153 | 0.076 |
| Methyl decanoate | 2.366 | 1.263 | 1.249 | 1.758 | 1.758 | 1.672 |
| Methyl nonanoate | 2.178 | 1.053 | 1.043 | 1.470 | 1.470 | 1.380 |
| Methyl Octanoate | 1.917 | 0.821 | 0.816 | 1.208 | 1.208 | 1.116 |
| Naphthalene | 1.041 | 0.986 | 0.961 | 1.291 | 1.291 | 1.302 |
| Nicotinamide | -3.146 | -4.190 | -3.878 | -3.367 | -3.367 | -4.255 |
| Nitrobenzene | 0.123 | 0.379 | 0.366 | 0.113 | 0.113 | 0.078 |
| Octanophenone | 1.915 | 1.013 | 1.005 | 1.491 | 1.491 | 1.363 |
| Pentachlorophenol | -0.607 | -0.251 | 0.016 | 0.740 | 0.740 | 0.626 |
| Perylene | 1.331 | 0.591 | 0.575 | 1.098 | 1.098 | 1.093 |
| Phenanthrene | 1.121 | 0.484 | 0.469 | 0.902 | 0.902 | 0.900 |
| Phenol | -2.460 | -1.340 | -1.126 | -1.020 | -1.020 | -1.305 |
| Phenylcyclohexane | 2.263 | 1.302 | 1.270 | 1.719 | 1.719 | 1.733 |
| Phthalonitrile | -0.842 | -1.425 | -1.395 | -1.929 | -1.929 | -2.044 |
| alpha-Pinene | 2.220 | 1.628 | 1.590 | 1.876 | 1.876 | 1.896 |
| beta-Pinene | 2.310 | 1.476 | 1.442 | 1.659 | 1.659 | 1.673 |
| Phenyl acetate | 0.215 | -0.456 | -0.442 | -0.227 | -0.227 | -0.312 |
| Phenyl benzoate | 1.009 | 0.096 | 0.096 | 0.448 | 0.448 | 0.380 |
| Phenylcyclohexane | 2.263 | 1.302 | 1.270 | 1.719 | 1.719 | 1.733 |
| n-Propylbenzene | 1.660 | 0.982 | 0.957 | 1.279 | 1.279 | 1.289 |
| Pyrene | 1.253 | 0.594 | 0.578 | 1.024 | 1.024 | 1.024 |
| Styrene | 1.145 | 0.386 | 0.374 | 0.666 | 0.666 | 0.666 |
| Terpinen-4-ol | 0.879 | 0.522 | 0.574 | 0.672 | 0.672 | 0.549 |
| Toluene | 0.994 | 1.424 | 1.392 | 1.686 | 1.686 | 1.707 |
| Tribenzylamine | 2.690 | 1.447 | 1.410 | 2.238 | 2.238 | 2.251 |
| Tri-n-butyrin | 1.504 | 0.049 | 0.069 | 0.520 | 0.520 | 0.348 |
| Triphenylene | 1.058 | 0.482 | 0.467 | 0.966 | 0.966 | 0.960 |
| Triphenylamine | 2.183 | 1.042 | 1.014 | 1.760 | 1.760 | 1.772 |
| Triphenylmethane | 2.308 | 3.045 | 2.978 | 3.838 | 3.838 | 3.884 |
| Valerophenone | 1.094 | 0.365 | 0.372 | 0.688 | 0.688 | 0.555 |
| Vanillin | -1.803 | -1.776 | -1.604 | -1.351 | -1.351 | -1.697 |

Table S10. Exp. and calculated log P for system n-heptane- ethanolamine at 25

°C

| Name | EXP | TZVP_ID | TZVP_EXP_M S | TZVPDFINE_E XP_MS | TZVPDFINE_P RED_FINE_MS | TZVPDFINE_P RED_TZVP_M S |
|----------------------------|--------|---------|-----------------|----------------------|----------------------------|--------------------------------|
| 1-Bromonaphthalene | 0.534 | -0.316 | -0.313 | 0.027 | 0.064 | -0.050 |
| 1-Methylnaphthalene | 0.596 | 0.237 | 0.238 | 0.624 | 0.563 | 0.481 |
| 1-Nitronaphthalene | -0.110 | -1.138 | -1.131 | -1.058 | -0.791 | -0.980 |
| 1,3-Dinitrobenzene | -0.961 | -1.911 | -1.901 | -2.039 | -1.493 | -1.744 |
| 1,2,4,5-Tetrachlorobenzene | 0.942 | -0.134 | -0.131 | 0.273 | 0.305 | 0.201 |
| 2-Chloroaniline | -0.902 | -1.764 | -1.750 | -1.487 | -1.189 | -1.379 |
| 2-Chlorophenol | -2.292 | -1.867 | -1.735 | -0.825 | -0.606 | -0.775 |
| 2-Methoxynaphthalene | 0.159 | -0.648 | -0.644 | -0.264 | -0.169 | -0.297 |
| 2-Methylnaphthalene | 0.623 | 0.317 | 0.317 | 0.719 | 0.640 | 0.559 |
| 2-Methylphenol | -2.824 | -1.362 | -1.302 | -1.173 | -0.671 | -0.937 |
| 2-Nitroaniline | -2.285 | -2.726 | -2.698 | -2.840 | -2.073 | -2.439 |
| 2-Nitrotoluene | 0.062 | -0.874 | -0.869 | -0.893 | -0.672 | -0.825 |
| 2-Phenylethanol | -1.924 | -1.743 | -1.639 | -1.326 | -0.618 | -0.957 |
| 2,5-Dichloroaniline | -1.250 | -2.012 | -1.992 | -1.680 | -1.322 | -1.553 |
| 3-Bromophenol | -4.039 | -4.041 | -3.403 | -3.046 | -1.496 | -1.939 |
| 3-Methylphenol | -3.066 | -3.551 | -3.076 | -2.735 | -1.360 | -1.782 |
| 3-Nitroaniline | -3.168 | -2.987 | -2.962 | -3.033 | -2.316 | -2.651 |

| | | | | | | |
|-----------------------------|--------|--------|--------|--------|--------|--------|
| 3-Nitrotoluene | 0.075 | -0.786 | -0.782 | -0.907 | -0.680 | -0.841 |
| 3-Phenylpropan-1-ol | -1.691 | -2.568 | -2.435 | -2.080 | -1.181 | -1.565 |
| 3,4-Dichloroaniline | -1.954 | -2.341 | -2.320 | -2.258 | -1.738 | -2.016 |
| 3,5-Dimethylphenol | -2.659 | -3.308 | -2.864 | -2.558 | -1.237 | -1.665 |
| 4-Chloroaniline | -1.798 | -2.182 | -2.165 | -1.994 | -1.541 | -1.770 |
| 4-Chlorophenol | -3.613 | -4.129 | -3.517 | -2.985 | -1.486 | -1.921 |
| 4-Methylphenol | -3.066 | -3.531 | -3.072 | -2.710 | -1.345 | -1.769 |
| 4-Nitrobenzyl alcohol | -2.939 | -3.844 | -3.582 | -3.459 | -2.096 | -2.573 |
| 4-Nitrotoluene | -0.030 | -0.874 | -0.870 | -1.070 | -0.806 | -0.980 |
| 4-Phenylphenol | -3.609 | -3.985 | -3.455 | -2.895 | -1.395 | -1.868 |
| Acenaphthylene | 0.329 | -0.460 | -0.456 | -0.052 | 0.011 | -0.108 |
| Acetanilide | -2.851 | -2.527 | -2.499 | -2.666 | -1.721 | -2.120 |
| Aniline | -1.727 | -0.522 | -0.516 | -0.418 | -0.311 | -0.434 |
| Anisole | 0.416 | -0.562 | -0.559 | -0.287 | -0.203 | -0.297 |
| Benzamide | -3.791 | -3.536 | -3.500 | -3.575 | -2.558 | -3.010 |
| Benzyl alcohol | -2.148 | -1.712 | -1.617 | -1.119 | -0.611 | -0.884 |
| Borneol | -0.213 | -1.216 | -1.145 | -1.068 | -0.525 | -0.826 |
| Carbazole | -2.009 | -2.090 | -2.060 | -1.825 | -1.187 | -1.545 |
| Chrysene | 0.527 | -0.719 | -0.714 | -0.129 | -0.012 | -0.194 |
| Decan-1-ol | 0.329 | -1.347 | -1.241 | -0.777 | -0.098 | -0.467 |
| Dibenzofuran | 0.448 | -0.513 | -0.509 | 0.028 | 0.067 | -0.048 |
| Dibenzylamine | 0.110 | -0.681 | -0.676 | -0.339 | -0.202 | -0.379 |
| Dibenzyl ether | 0.474 | -0.873 | -0.867 | -0.495 | -0.275 | -0.473 |
| Dicyclohexylamine | 1.813 | 0.494 | 0.496 | 0.753 | 0.689 | 0.561 |
| N,N-Diethylaniline | 0.807 | 0.798 | 0.798 | 1.112 | 0.960 | 0.886 |
| N,N-Diethylcarbanilide | 0.652 | -0.685 | -0.678 | -0.194 | 0.007 | -0.200 |
| N,N-Dimethylaniline | 0.110 | -0.341 | -0.338 | -0.217 | -0.130 | -0.241 |
| N,N-Dimethyl-4-nitroaniline | -0.514 | -1.695 | -1.686 | -3.127 | -2.313 | -2.694 |
| Diphenylamine | -0.609 | -1.408 | -1.394 | -1.096 | -0.769 | -1.014 |
| Diphenyl ether | 0.765 | -0.491 | -0.487 | 0.076 | 0.107 | -0.010 |
| Dodecane | 3.209 | 1.460 | 1.458 | 2.107 | 1.821 | 1.751 |
| Fluoranthene | 0.233 | -0.521 | -0.517 | 0.004 | 0.081 | -0.073 |
| Fluorene | 0.448 | -0.399 | -0.396 | 0.072 | 0.116 | -0.004 |
| Hexachlorobenzene | 1.304 | 0.466 | 0.466 | 0.820 | 0.721 | 0.641 |
| Hexan-1-ol | -0.908 | -1.831 | -1.723 | -1.418 | -0.702 | -1.034 |
| Indole | -2.363 | -2.282 | -2.248 | -1.963 | -1.362 | -1.680 |
| Iodobenzene | 0.375 | -0.335 | -0.332 | -0.086 | -0.045 | -0.137 |
| Limonene | 1.742 | 0.473 | 0.473 | 0.850 | 0.747 | 0.676 |
| Linalool | 0.272 | -0.019 | -0.016 | 0.214 | 0.263 | 0.149 |
| Nitrobenzene | -0.271 | -0.453 | -0.450 | -0.581 | -0.423 | -0.552 |
| Pentachlorophenol | -1.688 | -1.809 | -1.492 | -0.585 | -0.228 | -0.474 |
| Perylene | 0.634 | -0.733 | -0.727 | -0.133 | -0.006 | -0.202 |
| Phenanthrene | 0.491 | -0.548 | -0.544 | -0.054 | 0.025 | -0.116 |
| Pyrene | 0.409 | -0.498 | -0.494 | 0.015 | 0.085 | -0.063 |
| Quinoline | -0.254 | -0.892 | -0.885 | -0.796 | -0.566 | -0.728 |
| Terpinen-4-ol | 0.115 | -0.216 | -0.208 | -0.078 | 0.027 | -0.119 |
| Triphenylamine | 0.942 | -0.328 | -0.324 | 0.526 | 0.500 | 0.356 |
| n-Undecane | 2.878 | 1.346 | 1.343 | 1.937 | 1.672 | 1.607 |

Table S11: Experimental (this work) tie lines of the ternary systems involved in calculations for the system n-heptane/ethanol/ethylene glycol (37.5/25/37.5) at 25 °C

| Phase | n-heptane (%wt) | Ethanol (%wt) | Ethylene glycol (%wt) |
|---------------|-----------------|---------------|-----------------------|
| Bottom | 9.47 | 34.44 | 56.09 |
| Upper | 93.20 | 5.83 | 0.97 |

Table S12: Experimental (this work) tie lines of the ternary systems involved in calculations for the system n-heptane/ethanol/glycerol (37.5/25/37.5) at 25 °C

| Phase | n-heptane (%wt) | Ethanol (%wt) | Ethylene glycol (%wt) |
|---------------|------------------------|----------------------|------------------------------|
| Bottom | 2.84 | 36.39 | 60.77 |
| Upper | 93.76 | 4.92 | 1.32 |

Table S13: Experimental (this work) tie lines of the ternary systems involved in calculations for the system n-heptane/ethanol/levulinic acid (37.5/25/37.5) at 25 °C

| Phase | n-heptane (%wt) | Ethanol (%wt) | Ethylene glycol (%wt) |
|---------------|------------------------|----------------------|------------------------------|
| Bottom | 6.20 | 38.53 | 55.26 |
| Upper | 99.20 | 0.56 | 0.26 |