

# Benzoic acid, methyl ester

|                      |                                                                                                                                                                                                                              |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | CLORIUS<br>Essence of niobe<br>METHYL BENZENECARBOXYLATE<br>Methyl benzoate<br>Methyl ester of benzoic acid<br>Methylester kyseliny benzoove<br>NSC 9394<br>Niobe oil<br>Oil of Niobe<br>Oniobe oil<br>Oxidate le<br>UN 2938 |
| Inchi:               | InChI=1S/C8H8O2/c1-10-8(9)7-5-3-2-4-6-7/h2-6H,1H3                                                                                                                                                                            |
| InchiKey:            | QPJVMBTYPHYUOC-UHFFFAOYSA-N                                                                                                                                                                                                  |
| Formula:             | C8H8O2                                                                                                                                                                                                                       |
| SMILES:              | COC(=O)c1ccccc1                                                                                                                                                                                                              |
| Mol. weight [g/mol]: | 136.15                                                                                                                                                                                                                       |
| CAS:                 | 93-58-3                                                                                                                                                                                                                      |

## Physical Properties

| Property code | Value           | Unit   | Source        |
|---------------|-----------------|--------|---------------|
| af            | 0.4300          |        | KDB           |
| affp          | 850.50          | kJ/mol | NIST Webbook  |
| basg          | 814.90 ± 0.50   | kJ/mol | NIST Webbook  |
| basg          | 819.50          | kJ/mol | NIST Webbook  |
| chl           | -3947.90 ± 2.40 | kJ/mol | NIST Webbook  |
| dm            | 1.90            | debye  | KDB           |
| ea            | 0.18            | eV     | NIST Webbook  |
| gf            | -105.03         | kJ/mol | Joback Method |
| hf            | -269.30 ± 5.10  | kJ/mol | NIST Webbook  |
| hf            | -299.80         | kJ/mol | NIST Webbook  |
| hf            | -254.10         | kJ/mol | KDB           |
| hfl           | -324.30 ± 3.00  | kJ/mol | NIST Webbook  |
| hfl           | -343.50         | kJ/mol | NIST Webbook  |
| hfus          | 13.30           | kJ/mol | Joback Method |
| hvap          | 55.57 ± 0.04    | kJ/mol | NIST Webbook  |
| hvap          | 43.72           | kJ/mol | NIST Webbook  |

|         |                |        |                                                               |
|---------|----------------|--------|---------------------------------------------------------------|
| hvap    | 43.70          | kJ/mol | NIST Webbook                                                  |
| hvap    | 53.40          | kJ/mol | NIST Webbook                                                  |
| hvap    | 53.80          | kJ/mol | NIST Webbook                                                  |
| hvap    | 54.70          | kJ/mol | NIST Webbook                                                  |
| hvap    | 53.90          | kJ/mol | NIST Webbook                                                  |
| hvap    | 55.60 ± 0.10   | kJ/mol | NIST Webbook                                                  |
| hvap    | 55.00          | kJ/mol | NIST Webbook                                                  |
| ie      | 9.49           | eV     | NIST Webbook                                                  |
| ie      | 9.50           | eV     | NIST Webbook                                                  |
| ie      | 9.79           | eV     | NIST Webbook                                                  |
| ie      | 9.32 ± 0.04    | eV     | NIST Webbook                                                  |
| ie      | 9.32 ± 0.03    | eV     | NIST Webbook                                                  |
| ie      | 9.48           | eV     | NIST Webbook                                                  |
| ie      | 9.35 ± 0.06    | eV     | NIST Webbook                                                  |
| ie      | 9.40 ± 0.10    | eV     | NIST Webbook                                                  |
| ie      | 9.40 ± 0.03    | eV     | NIST Webbook                                                  |
| ie      | 9.35 ± 0.03    | eV     | NIST Webbook                                                  |
| ie      | 9.34           | eV     | NIST Webbook                                                  |
| ie      | 9.28           | eV     | NIST Webbook                                                  |
| log10ws | -1.85          |        | Estimated Solubility Method                                   |
| log10ws | -1.85          |        | Aqueous Solubility Prediction Method                          |
| logp    | 1.473          |        | Crippen Method                                                |
| mcvol   | 107.260        | ml/mol | McGowan Method                                                |
| nfpaf   | %!d(float64=2) |        | KDB                                                           |
| pc      | 3640.00        | kPa    | KDB                                                           |
| pc      | 3460.00        | kPa    | Critical Point Measurements for n-Alkyl Benzoates (C8 to C13) |
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| ripol | 1600.00       |         | NIST Webbook                            |
| ripol | 1614.00       |         | NIST Webbook                            |
| tb    | 472.20        | K       | KDB                                     |
| tc    | 692.00        | K       | KDB                                     |
| tf    | 260.94 ± 0.05 | K       | NIST Webbook                            |
| tf    | 260.80 ± 0.02 | K       | NIST Webbook                            |
| tf    | 260.70 ± 0.20 | K       | NIST Webbook                            |
| tf    | 260.80        | K       | NIST Webbook                            |
| tf    | 260.40        | K       | Aqueous Solubility<br>Prediction Method |
| tf    | 260.80        | K       | KDB                                     |
| tf    | 260.75 ± 0.30 | K       | NIST Webbook                            |
| vc    | 0.396         | m3/kmol | KDB                                     |
| zc    | 0.2505270     |         | KDB                                     |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|



|       |           |         |        |                                                                                                                                                                                                                            |
|-------|-----------|---------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cpg   | 225.73    | J/mol×K | 522.02 | Joback Method                                                                                                                                                                                                              |
| cpg   | 236.56    | J/mol×K | 558.64 | Joback Method                                                                                                                                                                                                              |
| cpg   | 246.75    | J/mol×K | 595.25 | Joback Method                                                                                                                                                                                                              |
| cpg   | 256.31    | J/mol×K | 631.87 | Joback Method                                                                                                                                                                                                              |
| cpg   | 265.28    | J/mol×K | 668.48 | Joback Method                                                                                                                                                                                                              |
| cpg   | 273.64    | J/mol×K | 705.10 | Joback Method                                                                                                                                                                                                              |
| cpg   | 214.26    | J/mol×K | 485.41 | Joback Method                                                                                                                                                                                                              |
| cpl   | 221.30    | J/mol×K | 298.15 | NIST Webbook                                                                                                                                                                                                               |
| cpl   | 216.50    | J/mol×K | 297.00 | NIST Webbook                                                                                                                                                                                                               |
| dvisc | 0.0018510 | Pa×s    | 298.15 | Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T ) (288.15, 298.15, 308.15, and 318.15) K |
| dvisc | 0.0012970 | Pa×s    | 318.15 | Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T ) (288.15, 298.15, 308.15, and 318.15) K |
| dvisc | 0.0017780 | Pa×s    | 303.15 | Density and Viscosity Studies of Binary Mixtures of N,N-Dimethylformamide with Toluene and Methyl Benzoate at (298.15, 303.15, 308.15, and 313.15) K                                                                       |
| dvisc | 0.0019180 | Pa×s    | 298.15 | Density and Viscosity Studies of Binary Mixtures of N,N-Dimethylformamide with Toluene and Methyl Benzoate at (298.15, 303.15, 308.15, and 313.15) K                                                                       |

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| dvisc | 0.0014020 | Pa×s | 313.15 | Density and Viscosity Studies of Binary Mixtures of N,N-Dimethylformamide with Toluene and Methyl Benzoate at (298.15, 303.15, 308.15, and 313.15) K                                                                       |
| dvisc | 0.0016790 | Pa×s | 303.15 | Thermophysical Properties of Isoamyl Acetate or Methyl Benzoate + Hydrocarbon Binary Mixtures, at (303.15 and 313.15) K                                                                                                    |
| dvisc | 0.0014140 | Pa×s | 313.15 | Thermophysical Properties of Isoamyl Acetate or Methyl Benzoate + Hydrocarbon Binary Mixtures, at (303.15 and 313.15) K                                                                                                    |
| dvisc | 0.0016670 | Pa×s | 303.15 | Density, Viscosity, and Speed of Sound of (Methyl Benzoate + Cyclohexane), (Methyl Benzoate + n-Hexane), (Methyl Benzoate + Heptane), and (Methyl Benzoate + Octane) at Temperatures of (303.15, 308.15, and 313.15) K     |
| dvisc | 0.0022970 | Pa×s | 288.15 | Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T ) (288.15, 298.15, 308.15, and 318.15) K |

|       |              |        |        |                                                                                                                                                                                                                            |
|-------|--------------|--------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dvisc | 0.0015140    | Pa×s   | 308.15 | Density, Viscosity, and Speed of Sound of (Methyl Benzoate + Cyclohexane), (Methyl Benzoate + n-Hexane), (Methyl Benzoate + Heptane), and (Methyl Benzoate + Octane) at Temperatures of (303.15, 308.15, and 313.15) K     |
| dvisc | 0.0013760    | Pa×s   | 313.15 | Density, Viscosity, and Speed of Sound of (Methyl Benzoate + Cyclohexane), (Methyl Benzoate + n-Hexane), (Methyl Benzoate + Heptane), and (Methyl Benzoate + Octane) at Temperatures of (303.15, 308.15, and 313.15) K     |
| dvisc | 0.0016630    | Pa×s   | 308.15 | Density and Viscosity Studies of Binary Mixtures of N,N-Dimethylformamide with Toluene and Methyl Benzoate at (298.15, 303.15, 308.15, and 313.15) K                                                                       |
| dvisc | 0.0015310    | Pa×s   | 308.15 | Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T ) (288.15, 298.15, 308.15, and 318.15) K |
| hfust | 13.90        | kJ/mol | 261.00 | NIST Webbook                                                                                                                                                                                                               |
| hfust | 14.83        | kJ/mol | 260.80 | NIST Webbook                                                                                                                                                                                                               |
| hfust | 14.80        | kJ/mol | 162.50 | NIST Webbook                                                                                                                                                                                                               |
| hfust | 13.90        | kJ/mol | 261.00 | NIST Webbook                                                                                                                                                                                                               |
| hvapt | 49.70        | kJ/mol | 453.00 | NIST Webbook                                                                                                                                                                                                               |
| hvapt | 45.80 ± 0.20 | kJ/mol | 437.50 | NIST Webbook                                                                                                                                                                                                               |
| hvapt | 43.00 ± 0.40 | kJ/mol | 437.50 | NIST Webbook                                                                                                                                                                                                               |

|       |              |        |        |                                                                                                                                                                                                                                      |
|-------|--------------|--------|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| hvapt | 57.20 ± 0.10 | kJ/mol | 303.00 | NIST Webbook                                                                                                                                                                                                                         |
| hvapt | 50.70        | kJ/mol | 381.00 | NIST Webbook                                                                                                                                                                                                                         |
| hvapt | 48.30        | kJ/mol | 381.00 | NIST Webbook                                                                                                                                                                                                                         |
| hvapt | 48.50 ± 0.20 | kJ/mol | 437.50 | NIST Webbook                                                                                                                                                                                                                         |
| hvapt | 52.80        | kJ/mol | 387.00 | NIST Webbook                                                                                                                                                                                                                         |
| hvapt | 51.10 ± 0.20 | kJ/mol | 437.50 | NIST Webbook                                                                                                                                                                                                                         |
| rhoI  | 1086.00      | kg/m3  | 293.00 | KDB                                                                                                                                                                                                                                  |
| rhoI  | 1077.00      | kg/m3  | 303.15 | Study of molecular interactions in the mixtures of some primary alcohols with equimolar mixture of 1-propanol and alkylbenzoates at T = 303.15 K                                                                                     |
| rhoI  | 1083.92      | kg/m3  | 298.15 | Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K |
| srf   | 0.04         | N/m    | 288.15 | Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T ) 288.15 K to T ) 358.15 K                                                                                                              |
| srf   | 0.03         | N/m    | 348.15 | Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T ) 288.15 K to T ) 358.15 K                                                                                                              |
| srf   | 0.04         | N/m    | 298.15 | Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T ) 288.15 K to T ) 358.15 K                                                                                                              |

|     |      |     |        |                                                                                                                                                 |
|-----|------|-----|--------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| srf | 0.04 | N/m | 308.15 | Densities,<br>Viscosities,<br>Refractive<br>Indices, and<br>Surface Tensions<br>for 12 Flavor<br>Esters from T )<br>288.15 K to T )<br>358.15 K |
| srf | 0.03 | N/m | 318.15 | Densities,<br>Viscosities,<br>Refractive<br>Indices, and<br>Surface Tensions<br>for 12 Flavor<br>Esters from T )<br>288.15 K to T )<br>358.15 K |
| srf | 0.03 | N/m | 328.15 | Densities,<br>Viscosities,<br>Refractive<br>Indices, and<br>Surface Tensions<br>for 12 Flavor<br>Esters from T )<br>288.15 K to T )<br>358.15 K |
| srf | 0.03 | N/m | 338.15 | Densities,<br>Viscosities,<br>Refractive<br>Indices, and<br>Surface Tensions<br>for 12 Flavor<br>Esters from T )<br>288.15 K to T )<br>358.15 K |
| srf | 0.03 | N/m | 358.15 | Densities,<br>Viscosities,<br>Refractive<br>Indices, and<br>Surface Tensions<br>for 12 Flavor<br>Esters from T )<br>288.15 K to T )<br>358.15 K |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 370.20        | K    | 3.20           | NIST Webbook |
| tbrp          | 370.00 ± 1.00 | K    | 3.20           | NIST Webbook |

# Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.48415e+01                   |
| Coeff. B                    | -4.20259e+03                  |
| Coeff. C                    | -6.15670e+01                  |
| Temperature range (K), min. | 350.33                        |
| Temperature range (K), max. | 502.55                        |

| Information                 | Value                                      |
|-----------------------------|--------------------------------------------|
| Property code               | pvap                                       |
| Equation                    | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A                    | 1.04360e+02                                |
| Coeff. B                    | -1.02686e+04                               |
| Coeff. C                    | -1.28853e+01                               |
| Coeff. D                    | 6.03145e-06                                |
| Temperature range (K), min. | 260.75                                     |
| Temperature range (K), max. | 693.00                                     |

# Datasets

## Mass density, kg/m3

| Temperature, K - Liquid | Pressure, kPa - Liquid | Mass density, kg/m3 - Liquid |
|-------------------------|------------------------|------------------------------|
| 278.15                  | 100.00                 | 1101.5                       |
| 278.15                  | 1000.00                | 1102.1                       |
| 278.15                  | 5000.00                | 1104.4                       |
| 278.15                  | 10000.00               | 1107.2                       |
| 278.15                  | 15000.00               | 1109.9                       |
| 278.15                  | 20000.00               | 1112.6                       |
| 278.15                  | 25000.00               | 1115.2                       |
| 278.15                  | 30000.00               | 1117.7                       |
| 278.15                  | 35000.00               | 1120.2                       |

|        |          |        |
|--------|----------|--------|
| 278.15 | 40000.00 | 1122.7 |
| 278.15 | 45000.00 | 1125.1 |
| 278.15 | 50000.00 | 1127.4 |
| 278.15 | 55000.00 | 1129.7 |
| 278.15 | 60000.00 | 1131.8 |
| 288.15 | 100.00   | 1092.1 |
| 288.15 | 1000.00  | 1092.6 |
| 288.15 | 5000.00  | 1095.0 |
| 288.15 | 10000.00 | 1097.9 |
| 288.15 | 15000.00 | 1100.8 |
| 288.15 | 20000.00 | 1103.6 |
| 288.15 | 25000.00 | 1106.3 |
| 288.15 | 30000.00 | 1109.0 |
| 288.15 | 35000.00 | 1111.6 |
| 288.15 | 40000.00 | 1114.1 |
| 288.15 | 45000.00 | 1116.6 |
| 288.15 | 50000.00 | 1119.1 |
| 288.15 | 55000.00 | 1121.4 |
| 288.15 | 60000.00 | 1123.6 |
| 298.15 | 100.00   | 1082.7 |
| 298.15 | 1000.00  | 1083.2 |
| 298.15 | 5000.00  | 1085.8 |
| 298.15 | 10000.00 | 1089.0 |
| 298.15 | 15000.00 | 1091.8 |
| 298.15 | 20000.00 | 1094.8 |
| 298.15 | 25000.00 | 1097.6 |
| 298.15 | 30000.00 | 1100.4 |
| 298.15 | 35000.00 | 1103.1 |
| 298.15 | 40000.00 | 1105.7 |
| 298.15 | 45000.00 | 1108.3 |
| 298.15 | 50000.00 | 1110.9 |
| 298.15 | 55000.00 | 1113.4 |
| 298.15 | 60000.00 | 1115.6 |
| 308.15 | 100.00   | 1073.0 |
| 308.15 | 1000.00  | 1073.6 |
| 308.15 | 5000.00  | 1076.2 |
| 308.15 | 10000.00 | 1079.5 |
| 308.15 | 15000.00 | 1082.6 |
| 308.15 | 20000.00 | 1085.7 |
| 308.15 | 25000.00 | 1088.6 |
| 308.15 | 30000.00 | 1091.5 |
| 308.15 | 35000.00 | 1094.3 |
| 308.15 | 40000.00 | 1097.1 |
| 308.15 | 45000.00 | 1099.8 |

|        |          |        |
|--------|----------|--------|
| 308.15 | 50000.00 | 1102.4 |
| 308.15 | 55000.00 | 1105.0 |
| 308.15 | 60000.00 | 1107.4 |
| 318.15 | 100.00   | 1063.3 |
| 318.15 | 1000.00  | 1063.8 |
| 318.15 | 5000.00  | 1066.7 |
| 318.15 | 10000.00 | 1070.1 |
| 318.15 | 15000.00 | 1073.4 |
| 318.15 | 20000.00 | 1076.6 |
| 318.15 | 25000.00 | 1079.7 |
| 318.15 | 30000.00 | 1082.8 |
| 318.15 | 35000.00 | 1085.7 |
| 318.15 | 40000.00 | 1088.6 |
| 318.15 | 45000.00 | 1091.4 |
| 318.15 | 50000.00 | 1094.1 |
| 318.15 | 55000.00 | 1096.8 |
| 318.15 | 60000.00 | 1099.3 |
| 328.15 | 100.00   | 1053.6 |
| 328.15 | 1000.00  | 1054.3 |
| 328.15 | 5000.00  | 1057.2 |
| 328.15 | 10000.00 | 1060.8 |
| 328.15 | 15000.00 | 1064.3 |
| 328.15 | 20000.00 | 1067.6 |
| 328.15 | 25000.00 | 1070.9 |
| 328.15 | 30000.00 | 1074.0 |
| 328.15 | 35000.00 | 1077.1 |
| 328.15 | 40000.00 | 1080.1 |
| 328.15 | 45000.00 | 1083.0 |
| 328.15 | 50000.00 | 1085.9 |
| 328.15 | 55000.00 | 1088.7 |
| 328.15 | 60000.00 | 1091.2 |
| 338.15 | 100.00   | 1044.1 |
| 338.15 | 1000.00  | 1044.8 |
| 338.15 | 5000.00  | 1048.0 |
| 338.15 | 10000.00 | 1051.7 |
| 338.15 | 15000.00 | 1055.3 |
| 338.15 | 20000.00 | 1058.8 |
| 338.15 | 25000.00 | 1062.2 |
| 338.15 | 30000.00 | 1065.5 |
| 338.15 | 35000.00 | 1068.8 |
| 338.15 | 40000.00 | 1071.9 |
| 338.15 | 45000.00 | 1074.9 |
| 338.15 | 50000.00 | 1077.9 |
| 338.15 | 55000.00 | 1080.8 |





|                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                   |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b>                                                                                                                                                                                                                                                                              | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                                         |
| <b>Joback Method:</b>                                                                                                                                                                                                                                                                               | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                             |
| <b>Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Benzoate, Methyl Benzoate, Benzyl Acetoacetate, Methyl Benzoate, Benzyl Acetoacetate, and Ethyl Benzoate with Ethanol at 288.15, 298.15, 308.15, and 318.15) K:</b>                                                    | <a href="https://www.doi.org/10.1021/je050402s">https://www.doi.org/10.1021/je050402s</a>                                                                                                         |
| <b>McGowan Method:</b>                                                                                                                                                                                                                                                                              | <a href="https://www.doi.org/10.1016/j.jct.2018.07.021">https://www.doi.org/10.1016/j.jct.2018.07.021</a>                                                                                         |
| <b>Compressed liquid density measurements for (methylbenzoate + toluene) and (ethylbenzoate + toluene) binary systems of Binary Mixtures of Ethyl Acetoacetate, Ethyl Benzoate, Methyl Benzoate, Ethyl Benzoate, and Benzyl Acetoacetate with Ethanol at 288.15, 298.15, 308.15, and 318.15) K:</b> | <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a> |
| <b>Refractive Indices and Surface Tension of Binary Mixtures of Ethyl Acetoacetate, Ethyl Benzoate, Methyl Benzoate, Ethyl Benzoate, and Benzyl Acetoacetate with Ethanol at 288.15, 298.15, 308.15, and 318.15) K:</b>                                                                             | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                             |
| <b>Aqueous Solubility Prediction Method:</b>                                                                                                                                                                                                                                                        | <a href="https://www.doi.org/10.1016/j.jct.2011.02.008">https://www.doi.org/10.1016/j.jct.2011.02.008</a>                                                                                         |
| <b>KDB:</b>                                                                                                                                                                                                                                                                                         | <a href="https://www.doi.org/10.1021/je060139a">https://www.doi.org/10.1021/je060139a</a>                                                                                                         |

## Legend

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                           |
| <b>affp:</b>    | Proton affinity                                           |
| <b>basg:</b>    | Gas basicity                                              |
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                   |
| <b>cpl:</b>     | Liquid phase heat capacity                                |
| <b>dm:</b>      | Dipole Moment                                             |
| <b>dvisc:</b>   | Dynamic viscosity                                         |
| <b>ea:</b>      | Electron affinity                                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation                   |
| <b>hf:</b>      | Enthalpy of formation at standard conditions              |
| <b>hfl:</b>     | Liquid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions                 |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature                 |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions           |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature           |
| <b>ie:</b>      | Ionization energy                                         |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l                        |
| <b>logp:</b>    | Octanol/Water partition coefficient                       |
| <b>mcvol:</b>   | McGowan's characteristic volume                           |
| <b>nfpaf:</b>   | NFPA Fire Rating                                          |
| <b>pc:</b>      | Critical Pressure                                         |
| <b>pvap:</b>    | Vapor pressure                                            |
| <b>rho:</b>     | Liquid Density                                            |

|                |                                   |
|----------------|-----------------------------------|
| <b>rinpol:</b> | Non-polar retention indices       |
| <b>ripol:</b>  | Polar retention indices           |
| <b>srf:</b>    | Surface Tension                   |
| <b>tb:</b>     | Normal Boiling Point Temperature  |
| <b>tbrp:</b>   | Boiling point at reduced pressure |
| <b>tc:</b>     | Critical Temperature              |
| <b>tf:</b>     | Normal melting (fusion) point     |
| <b>vc:</b>     | Critical Volume                   |
| <b>zc:</b>     | Critical Compressibility          |

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