# Benzene, tert-butyl-

| | |
|---|---|
| **Other names:** | (1,1-dimethylethyl)benzene |
| | 1,1-Dimethylethyl-benzene |
| | 2-METHYL-2-PHENYLPROPANE |
| | 2-PHENYL-2-METHYLPROPANE |
| | Benzene, (1,1-dimethylethyl)- |
| | Benzene, t-butyl- |
| | DIMETHYLETHYLBENZENE |
| | NSC 6557 |
| | Phenyltrimethylmethane |
| | Pseudobutylbenzene |
| | Trimethylphenylmethane |
| | benzene, 1,1-dimethylethyl- |
| | t-Butylbenzene |
| | tert-Butylbenzene |
| | «alpha»-dimethylethylbenzene |
| | Â«alphaÂ»-dimethylethylbenzene |
| **Inchi:** | InChI=1S/C10H14/c1-10(2,3)9-7-5-4-6-8-9/h4-8H,1-3H3 |
| **InchiKey:** | YTZKOQUCBOVLHL-UHFFFAOYSA-N |
| **Formula:** | C10H14 |
| **SMILES:** | CC(C)(C)c1ccccc1 |
| **Mol. weight [g/mol]:** | 134.22 |
| **CAS:** | 98-06-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.2650 | | KDB |
| chl | -5859.60 | kJ/mol | NIST Webbook |
| chl | -5865.20 ± 1.10 | kJ/mol | NIST Webbook |
| chl | -5856.76 | kJ/mol | NIST Webbook |
| dm | 0.50 | debye | KDB |
| gf | 148.57 | kJ/mol | Joback Method |
| hcg | 5867.22 | kJ/mol | KDB |
| hcn | 5559.700 | kJ/mol | KDB |
| hf | -22.70 ± 1.40 | kJ/mol | NIST Webbook |
| hf | -22.69 | kJ/mol | KDB |
| hfl | -70.80 ± 1.30 | kJ/mol | NIST Webbook |

| | | | |
|---|---|---|---|
| hfus | 8.39 | kJ/mol | Thermodynamic properties of tert-butylbenzene and 1,4-di-tert-butylbenzene |
| hvap | 38.83 | kJ/mol | Joback Method |
| ie | 8.25 | eV | NIST Webbook |
| ie | 8.68 ± 0.01 | eV | NIST Webbook |
| ie | 8.68 ± 0.01 | eV | NIST Webbook |
| ie | 8.81 | eV | NIST Webbook |
| ie | 8.65 | eV | NIST Webbook |
| ie | 8.69 | eV | NIST Webbook |
| ie | 8.63 ± 0.01 | eV | NIST Webbook |
| ie | 8.74 ± 0.05 | eV | NIST Webbook |
| ie | 8.69 | eV | NIST Webbook |
| ie | 8.68 ± 0.03 | eV | NIST Webbook |
| ie | 8.83 | eV | NIST Webbook |
| ie | 8.64 | eV | NIST Webbook |
| ie | 8.72 ± 0.01 | eV | NIST Webbook |
| log10ws | -3.66 | | Estimated Solubility Method |
| log10ws | -3.66 | | Aqueous Solubility Prediction Method |
| logp | 2.984 | | Crippen Method |
| mcvol | 128.000 | ml/mol | McGowan Method |
| pc | 2960.00 | kPa | KDB |
| rinpol | 976.53 | | NIST Webbook |
| rinpol | 993.50 | | NIST Webbook |
| rinpol | 1000.90 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 969.90 | | NIST Webbook |
| rinpol | 969.90 | | NIST Webbook |
| rinpol | 972.50 | | NIST Webbook |
| rinpol | 972.00 | | NIST Webbook |
| rinpol | 967.08 | | NIST Webbook |
| rinpol | 975.40 | | NIST Webbook |
| rinpol | 973.30 | | NIST Webbook |
| rinpol | 976.00 | | NIST Webbook |
| rinpol | 992.00 | | NIST Webbook |
| rinpol | 983.22 | | NIST Webbook |
| rinpol | 981.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 987.10 | | NIST Webbook |
| rinpol | 990.50 | | NIST Webbook |
| rinpol | 992.00 | | NIST Webbook |
| rinpol | 972.40 | | NIST Webbook |
| rinpol | 979.30 | | NIST Webbook |
| rinpol | 979.10 | | NIST Webbook |

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|---|---|---|
| rinpol | 987.10 | NIST Webbook |
| rinpol | 990.50 | NIST Webbook |
| rinpol | 992.00 | NIST Webbook |
| rinpol | 978.00 | NIST Webbook |
| rinpol | 988.00 | NIST Webbook |
| rinpol | 972.82 | NIST Webbook |
| rinpol | 987.60 | NIST Webbook |
| rinpol | 978.96 | NIST Webbook |
| rinpol | 989.31 | NIST Webbook |
| rinpol | 993.20 | NIST Webbook |
| rinpol | 995.68 | NIST Webbook |
| rinpol | 976.00 | NIST Webbook |
| rinpol | 1001.00 | NIST Webbook |
| rinpol | 988.00 | NIST Webbook |
| rinpol | 963.00 | NIST Webbook |
| rinpol | 976.00 | NIST Webbook |
| rinpol | 994.00 | NIST Webbook |
| rinpol | 972.50 | NIST Webbook |
| rinpol | 984.00 | NIST Webbook |
| rinpol | 984.00 | NIST Webbook |
| rinpol | 984.00 | NIST Webbook |
| rinpol | 975.00 | NIST Webbook |
| rinpol | 994.00 | NIST Webbook |
| rinpol | 971.00 | NIST Webbook |
| rinpol | 975.00 | NIST Webbook |
| rinpol | 975.00 | NIST Webbook |
| rinpol | 980.00 | NIST Webbook |
| rinpol | 961.00 | NIST Webbook |
| rinpol | 988.00 | NIST Webbook |
| rinpol | 973.00 | NIST Webbook |
| rinpol | 986.00 | NIST Webbook |
| rinpol | 991.00 | NIST Webbook |
| rinpol | 986.40 | NIST Webbook |
| rinpol | 993.80 | NIST Webbook |
| rinpol | 991.70 | NIST Webbook |
| rinpol | 991.90 | NIST Webbook |
| rinpol | 973.30 | NIST Webbook |
| rinpol | 1008.00 | NIST Webbook |
| rinpol | 985.00 | NIST Webbook |
| rinpol | 1000.00 | NIST Webbook |
| rinpol | 971.00 | NIST Webbook |
| rinpol | 969.90 | NIST Webbook |
| rinpol | 1001.00 | NIST Webbook |
| rinpol | 994.00 | NIST Webbook |

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|---|---|---|---|
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 1008.00 | | NIST Webbook |
| rinpol | 980.00 | | NIST Webbook |
| rinpol | 975.40 | | NIST Webbook |
| rinpol | 974.90 | | NIST Webbook |
| rinpol | 971.00 | | NIST Webbook |
| rinpol | 974.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 1010.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 980.90 | | NIST Webbook |
| rinpol | 992.50 | | NIST Webbook |
| rinpol | 986.90 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 1008.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 977.00 | | NIST Webbook |
| ripol | 1229.50 | | NIST Webbook |
| ripol | 1287.00 | | NIST Webbook |
| ripol | 1229.00 | | NIST Webbook |
| ripol | 1262.00 | | NIST Webbook |
| ripol | 1215.00 | | NIST Webbook |
| ripol | 1247.00 | | NIST Webbook |
| ripol | 1215.00 | | NIST Webbook |
| ripol | 1223.00 | | NIST Webbook |
| ripol | 1251.00 | | NIST Webbook |
| ripol | 1237.50 | | NIST Webbook |
| ripol | 1275.00 | | NIST Webbook |
| ripol | 1249.00 | | NIST Webbook |
| ripol | 1215.10 | | NIST Webbook |
| ripol | 1239.00 | | NIST Webbook |
| sl | 278.70 | J/mol×K | NIST Webbook |
| tb | 442.30 | K | KDB |
| tc | 660.00 | K | KDB |
| tf | 215.30 | K | KDB |
| tf | 214.82 | K | Aqueous Solubility Prediction Method |
| tt | 215.00 ± 0.20 | K | NIST Webbook |
| vc | 0.476 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 258.79 | J/mol×K | 451.65 | Joback Method |
| cpg | 275.46 | J/mol×K | 488.10 | Joback Method |
| cpg | 343.10 | J/mol×K | 670.33 | Joback Method |
| cpg | 331.46 | J/mol×K | 633.88 | Joback Method |
| cpg | 318.94 | J/mol×K | 597.44 | Joback Method |
| cpg | 305.47 | J/mol×K | 560.99 | Joback Method |
| cpg | 290.99 | J/mol×K | 524.54 | Joback Method |
| cpl | 238.11 | J/mol×K | 294.30 | NIST Webbook |
| dvisc | 0.0004458 | Pa×s | 378.20 | Joback Method |
| dvisc | 0.0011790 | Pa×s | 304.75 | Joback Method |
| dvisc | 0.0006880 | Pa×s | 341.48 | Joback Method |
| dvisc | 0.0002313 | Pa×s | 451.65 | Joback Method |
| dvisc | 0.0003119 | Pa×s | 414.92 | Joback Method |
| dvisc | 0.0023414 | Pa×s | 268.02 | Joback Method |
| dvisc | 0.0057820 | Pa×s | 231.30 | Joback Method |
| hfust | 8.41 | kJ/mol | 215.00 | NIST Webbook |
| hfust | 8.40 | kJ/mol | 215.00 | NIST Webbook |
| hfust | 8.40 | kJ/mol | 215.00 | NIST Webbook |
| hfust | 8.40 | kJ/mol | 215.30 | NIST Webbook |
| hvapt | 43.70 | kJ/mol | 400.00 | NIST Webbook |
| hvapt | 39.90 ± 0.30 | kJ/mol | 409.00 | NIST Webbook |
| hvapt | 37.00 ± 0.50 | kJ/mol | 409.00 | NIST Webbook |
| hvapt | 47.80 ± 0.40 | kJ/mol | 293.00 | NIST Webbook |
| hvapt | 43.10 | kJ/mol | 406.00 | NIST Webbook |
| hvapt | 45.30 ± 0.20 | kJ/mol | 409.00 | NIST Webbook |
| hvapt | 42.60 ± 0.20 | kJ/mol | 409.00 | NIST Webbook |
| rfi | 1.48007 | | 318.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |

| | | | |
|---|---|---|---|
| rfi | 1.49003 | 298.15 | Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons |
| rfi | 1.49009 | 298.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |
| rfi | 1.49018 | 298.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |
| rfi | 1.48763 | 303.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |
| rfi | 1.48509 | 308.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |

| | | | | |
|---|---|---|---|---|
| rfi | 1.48256 | | 313.15 | Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene and nitrobenzene at T = (298.15-318.15) K |
| rfi | 1.49024 | | 298.15 | KDB |
| rhol | 867.00 | kg/m3 | 293.00 | KDB |
| rhol | 862.23 | kg/m3 | 298.15 | Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies |
| rhol | 854.12 | kg/m3 | 308.15 | The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K |
| rhol | 849.98 | kg/m3 | 313.15 | The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K |
| rhol | 845.87 | kg/m3 | 318.15 | The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K |
| rhol | 841.72 | kg/m3 | 323.15 | The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K |

| | | | | |
|---|---|---|---|---|
| rhol | 862.28 | kg/m3 | 298.15 | The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K |
| sfust | 39.06 | J/mol×K | 215.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.38431e+01 |
| Coeff. B | -3.47592e+03 |
| Coeff. C | -6.54960e+01 |
| Temperature range (K), min. | 321.92 |
| Temperature range (K), max. | 472.91 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 9.26802e+01 |
| Coeff. B | -8.94559e+03 |
| Coeff. C | -1.13016e+01 |
| Coeff. D | 5.13608e-06 |
| Temperature range (K), min. | 215.27 |
| Temperature range (K), max. | 660.00 |

# Datasets

## Mass density, kg/m3

| Temperature, K - Liquid | Pressure, kPa - Liquid | Mass density, kg/m3 - Liquid |
|---|---|---|
| 298.15 | 100.00 | 862.38 |

| | | |
|---|---|---|
| 313.15 | 100.00 | 849.98 |
| 333.15 | 100.00 | 833.32 |
| 353.15 | 100.00 | 816.42 |
| 373.15 | 100.00 | 799.33 |
| 393.15 | 100.00 | 781.81 |
| 413.15 | 100.00 | 763.74 |
| 433.15 | 100.00 | 745.23 |
| 298.15 | 20100.00 | 875.86 |
| 313.15 | 20100.00 | 864.52 |
| 333.15 | 20100.00 | 849.54 |
| 353.15 | 20100.00 | 834.5 |
| 373.15 | 20100.00 | 819.57 |
| 393.15 | 20100.00 | 804.5 |
| 413.15 | 20100.00 | 789.38 |
| 433.15 | 20100.00 | 774.28 |
| 298.15 | 40100.00 | 887.54 |
| 313.15 | 40100.00 | 877.0 |
| 333.15 | 40100.00 | 863.16 |
| 353.15 | 40100.00 | 849.4 |
| 373.15 | 40100.00 | 835.86 |
| 393.15 | 40100.00 | 822.33 |
| 413.15 | 40100.00 | 808.84 |
| 433.15 | 40100.00 | 795.55 |
| 298.15 | 60100.00 | 897.94 |
| 313.15 | 60100.00 | 888.01 |
| 333.15 | 60100.00 | 875.06 |
| 353.15 | 60100.00 | 862.22 |
| 373.15 | 60100.00 | 849.64 |
| 393.15 | 60100.00 | 837.18 |
| 413.15 | 60100.00 | 824.82 |
| 433.15 | 60100.00 | 812.75 |
| 298.15 | 80100.00 | 907.35 |
| 313.15 | 80100.00 | 897.93 |
| 333.15 | 80100.00 | 885.65 |
| 353.15 | 80100.00 | 873.52 |
| 373.15 | 80100.00 | 861.72 |
| 393.15 | 80100.00 | 850.05 |
| 413.15 | 80100.00 | 838.52 |
| 433.15 | 80100.00 | 827.29 |
| 298.15 | 100100.00 | 915.98 |
| 313.15 | 100100.00 | 906.96 |
| 333.15 | 100100.00 | 895.25 |
| 353.15 | 100100.00 | 883.72 |
| 373.15 | 100100.00 | 872.52 |

| | | |
|---|---|---|
| 393.15 | 100100.00 | 861.47 |
| 413.15 | 100100.00 | 850.58 |
| 433.15 | 100100.00 | 840.05 |

Reference *https://www.doi.org/10.1016/j.fluid.2018.02.008*

## Speed of sound, m/s

| Temperature, K - Liquid | Pressure, kPa - Liquid | Speed of sound, m/s - Liquid |
|---|---|---|
| 298.15 | 100.00 | 1316.4 |
| 313.15 | 100.00 | 1255.3 |
| 333.15 | 100.00 | 1176.9 |
| 353.15 | 100.00 | 1101.8 |
| 373.15 | 100.00 | 1029.9 |
| 393.15 | 100.00 | 959.3 |
| 413.15 | 100.00 | 890.9 |
| 433.15 | 100.00 | 823.7 |
| 298.15 | 20100.00 | 1415.8 |
| 313.15 | 20100.00 | 1360.3 |
| 333.15 | 20100.00 | 1290.1 |
| 353.15 | 20100.00 | 1223.5 |
| 373.15 | 20100.00 | 1161.2 |
| 393.15 | 20100.00 | 1101.1 |
| 413.15 | 20100.00 | 1042.6 |
| 433.15 | 20100.00 | 987.2 |
| 298.15 | 40100.00 | 1501.7 |
| 313.15 | 40100.00 | 1450.3 |
| 333.15 | 40100.00 | 1385.4 |
| 353.15 | 40100.00 | 1324.4 |
| 373.15 | 40100.00 | 1267.7 |
| 393.15 | 40100.00 | 1213.3 |
| 413.15 | 40100.00 | 1161.1 |
| 433.15 | 40100.00 | 1112.1 |
| 298.15 | 60100.00 | 1578.5 |
| 313.15 | 60100.00 | 1529.8 |
| 333.15 | 60100.00 | 1469.0 |
| 353.15 | 60100.00 | 1411.8 |
| 373.15 | 60100.00 | 1359.0 |
| 393.15 | 60100.00 | 1308.5 |
| 413.15 | 60100.00 | 1260.2 |
| 433.15 | 60100.00 | 1215.1 |

| | | |
|---|---|---|
| 298.15 | 80100.00 | 1647.9 |
| 313.15 | 80100.00 | 1601.7 |
| 333.15 | 80100.00 | 1543.9 |
| 353.15 | 80100.00 | 1489.6 |
| 373.15 | 80100.00 | 1439.6 |
| 393.15 | 80100.00 | 1392.0 |
| 413.15 | 80100.00 | 1346.6 |
| 433.15 | 80100.00 | 1304.3 |
| 298.15 | 100100.00 | 1711.7 |
| 313.15 | 100100.00 | 1667.3 |
| 333.15 | 100100.00 | 1612.5 |
| 353.15 | 100100.00 | 1560.2 |
| 373.15 | 100100.00 | 1512.4 |
| 393.15 | 100100.00 | 1466.9 |
| 413.15 | 100100.00 | 1423.8 |
| 433.15 | 100100.00 | 1383.6 |

Reference *https://www.doi.org/10.1016/j.jct.2019.03.005*

# Sources

**The physicochemical properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane with various aromatic hydrocarbons at T = (308.15 to 323.15) K:** https://www.doi.org/10.1016/j.jct.2015.12.025

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol668.mol

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons:** https://www.doi.org/10.1007/s10765-005-8096-3

**Determination of Henry's Law Constants Using Internal Standards and Benchmark Values:** https://www.doi.org/10.1021/je3010535

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Liquid density measurements of cumene, tert-butylbenzene, and hexadecane over wide ranges of temperature and pressure:** https://www.doi.org/10.1016/j.fluid.2018.02.008

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C98066&Units=SI

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**KDB Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=668

**Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures 1. Excess and solvation enthalpies:** https://www.doi.org/10.1016/j.fluid.2006.10.013

**Volumetric and refractive properties of 1,3,5,7-tetravinyl-1,3,5,7-tetramethylcyclotetrasiloxane with methoxybenzene, chlorobenzene, tert-butylbenzene, and nitrobenzene at T = (298.15 to 318.15) K:** https://www.doi.org/10.1016/j.jct.2018.09.021

**Thermodynamic properties of cumene, tert-butylbenzene, and n-hexadecane:** https://www.doi.org/10.1016/j.jct.2019.03.005

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Saturated Heat Capacities of Some Linear and Branched Alkylbenzenes between (332 and 401) K:** https://www.doi.org/10.1021/je050273f

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

**Thermochemistry of ionic liquid-catalysed reactions. Isomerisation and transalkylation of tert-alkylbenzenes. Are these systems ideal?:** https://www.doi.org/10.1016/j.jct.2010.01.006

**Thermodynamic properties of tert-butylbenzene and 1-tert-butylnaphthalene:** https://www.doi.org/10.1016/j.jct.2008.10.008

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dm:** | Dipole Moment |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hcg:** | Heat of Combustion, Gross form |
| **hcn:** | Heat of Combustion, Net Form |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rfi:** | Refractive Index |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **speedsl:** | Speed of sound in fluid |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |

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