# 1-Butanethiol

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|---|---|
| **Other names:** | 1-Butyl mercaptan |
| | 1-Mercaptobutane |
| | 1-butylthiol |
| | Butanethiol |
| | Butyl mercaptan |
| | Butylthiol |
| | NCI-C60866 |
| | Thiobutyl alcohol |
| | butane-1-thiol |
| | n-Butanethiol |
| | n-Butyl mercaptan |
| | n-Butyl thioalcohol |
| | n-Butylthiol |
| | n-C4H9SH |
| **Inchi:** | InChI=1S/C4H10S/c1-2-3-4-5/h5H,2-4H2,1H3 |
| **InchiKey:** | WQAQPCDUOCURKW-UHFFFAOYSA-N |
| **Formula:** | C4H10S |
| **SMILES:** | CCCCS |
| **Mol. weight [g/mol]:** | 90.19 |
| **CAS:** | 109-79-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 801.70 | kJ/mol | NIST Webbook |
| basg | 770.50 | kJ/mol | NIST Webbook |
| gf | 12.19 | kJ/mol | Joback Method |
| hf | -87.41 | kJ/mol | Joback Method |
| hfus | 10.16 | kJ/mol | Joback Method |
| hvap | 36.60 ± 0.40 | kJ/mol | NIST Webbook |
| hvap | 36.50 | kJ/mol | NIST Webbook |
| hvap | 36.70 | kJ/mol | NIST Webbook |
| ie | 9.14 ± 0.01 | eV | NIST Webbook |
| ie | 9.14 ± 0.02 | eV | NIST Webbook |
| ie | 9.15 | eV | NIST Webbook |
| log10ws | -2.18 | | Aqueous Solubility Prediction Method |

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|---|---|---|---|
| log10ws | -2.18 | | Estimated Solubility Method |
| logp | 1.716 | | Crippen Method |
| mcvol | 83.570 | ml/mol | McGowan Method |
| nfpaf | %!d(float64=3) | | KDB |
| nfpah | %!d(float64=2) | | KDB |
| pc | 4227.54 | kPa | Joback Method |
| rhoc | 277.78 ± 6.31 | kg/m3 | NIST Webbook |
| rinpol | 722.00 | | NIST Webbook |
| rinpol | 721.30 | | NIST Webbook |
| rinpol | 729.70 | | NIST Webbook |
| rinpol | 714.80 | | NIST Webbook |
| rinpol | 716.90 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 692.00 | | NIST Webbook |
| rinpol | 713.00 | | NIST Webbook |
| rinpol | 716.60 | | NIST Webbook |
| rinpol | 705.00 | | NIST Webbook |
| rinpol | 677.00 | | NIST Webbook |
| rinpol | 718.00 | | NIST Webbook |
| rinpol | 742.00 | | NIST Webbook |
| rinpol | 717.00 | | NIST Webbook |
| rinpol | 726.00 | | NIST Webbook |
| rinpol | 715.00 | | NIST Webbook |
| rinpol | 721.00 | | NIST Webbook |
| rinpol | 699.00 | | NIST Webbook |
| rinpol | 726.00 | | NIST Webbook |
| rinpol | 718.00 | | NIST Webbook |
| rinpol | 703.00 | | NIST Webbook |
| rinpol | 713.00 | | NIST Webbook |
| rinpol | 693.00 | | NIST Webbook |
| rinpol | 701.00 | | NIST Webbook |
| rinpol | 673.00 | | NIST Webbook |
| rinpol | 701.00 | | NIST Webbook |
| rinpol | 724.00 | | NIST Webbook |
| rinpol | 693.00 | | NIST Webbook |
| rinpol | 691.00 | | NIST Webbook |
| rinpol | 718.90 | | NIST Webbook |
| ripol | 944.00 | | NIST Webbook |
| ripol | 944.00 | | NIST Webbook |
| ripol | 919.00 | | NIST Webbook |
| ripol | 960.00 | | NIST Webbook |
| ripol | 938.00 | | NIST Webbook |
| ripol | 938.00 | | NIST Webbook |
| sl | 275.98 | J/mol×K | NIST Webbook |

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|---|---|---|---|
| tb | 371.60 | K | KDB |
| tb | 371.00 ± 3.00 | K | NIST Webbook |
| tb | 370.40 ± 1.50 | K | NIST Webbook |
| tb | 371.00 ± 3.00 | K | NIST Webbook |
| tb | 370.70 ± 0.70 | K | NIST Webbook |
| tb | 370.70 ± 0.50 | K | NIST Webbook |
| tb | 371.73 ± 0.25 | K | NIST Webbook |
| tb | 372.00 ± 3.00 | K | NIST Webbook |
| tb | 370.20 ± 0.30 | K | NIST Webbook |
| tb | 371.00 ± 3.00 | K | NIST Webbook |
| tb | 371.73 ± 0.40 | K | NIST Webbook |
| tb | 369.00 ± 4.00 | K | NIST Webbook |
| tb | 369.00 ± 3.00 | K | NIST Webbook |
| tb | 371.20 ± 0.40 | K | NIST Webbook |
| tb | 370.00 ± 2.00 | K | NIST Webbook |
| tb | 371.60 | K | NIST Webbook |
| tb | 371.00 | K | NIST Webbook |
| tb | 371.60 | K | NIST Webbook |
| tb | 371.30 ± 1.00 | K | NIST Webbook |
| tb | 370.00 ± 2.00 | K | NIST Webbook |
| tc | 570.10 | K | KDB |
| tc | 570.10 ± 0.40 | K | NIST Webbook |
| tc | 569.20 | K | NIST Webbook |
| tf | 157.48 ± 0.07 | K | NIST Webbook |
| tf | 157.03 ± 0.25 | K | NIST Webbook |
| tf | 157.30 ± 0.50 | K | NIST Webbook |
| tf | 157.40 | K | KDB |
| tf | 157.23 | K | Aqueous Solubility Prediction Method |
| tf | 157.30 ± 0.30 | K | NIST Webbook |
| tt | 157.47 ± 0.05 | K | NIST Webbook |
| tt | 157.46 | K | KDB |
| vc | 0.324 | m3/kmol | KDB |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 142.92 | J/mol×K | 385.55 | Joback Method |
| cpg | 151.11 | J/mol×K | 417.32 | Joback Method |
| cpg | 158.97 | J/mol×K | 449.09 | Joback Method |
| cpg | 166.51 | J/mol×K | 480.86 | Joback Method |

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|---|---|---|---|---|
| cpg | 173.74 | J/mol×K | 512.63 | Joback Method |
| cpg | 180.66 | J/mol×K | 544.40 | Joback Method |
| cpg | 134.39 | J/mol×K | 353.78 | Joback Method |
| cpl | 172.30 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 171.39 | J/mol×K | 300.00 | NIST Webbook |
| hfust | 10.46 | kJ/mol | 157.47 | NIST Webbook |
| hfust | 10.46 | kJ/mol | 157.50 | NIST Webbook |
| hfust | 10.46 | kJ/mol | 157.50 | NIST Webbook |
| hvapt | 32.20 ± 0.10 | kJ/mol | 371.00 | NIST Webbook |
| hvapt | 33.60 ± 0.10 | kJ/mol | 350.00 | NIST Webbook |
| hvapt | 34.70 ± 0.10 | kJ/mol | 330.00 | NIST Webbook |
| hvapt | 35.00 | kJ/mol | 366.00 | NIST Webbook |
| hvapt | 32.23 | kJ/mol | 371.60 | NIST Webbook |
| pvap | 40.90 | kPa | 343.41 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 91.60 | kPa | 368.05 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 81.90 | kPa | 364.39 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 72.60 | kPa | 360.57 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 61.90 | kPa | 355.65 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 52.10 | kPa | 350.44 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |

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|---|---|---|---|---|
| pvap | 31.40 | kPa | 336.10 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 23.10 | kPa | 328.08 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| pvap | 100.50 | kPa | 371.04 | Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons |
| sfust | 66.43 | J/mol×K | 157.47 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.54429e+01 |
| Coeff. B | -3.53467e+03 |
| Coeff. C | -4.44580e+01 |
| Temperature range (K), min. | 277.69 |
| Temperature range (K), max. | 393.34 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.14838e+01 |
| Coeff. B | -7.01146e+03 |
| Coeff. C | -9.97282e+00 |
| Coeff. D | 7.38659e-06 |
| Temperature range (K), min. | 157.46 |
| Temperature range (K), max. | 569.00 |

# Sources

| | |
|---|---|
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Phase Equilibrium Measurements and Modeling of 1-Propanethiol + Ethanethiol + CH4 in Methane Ternary System at 303.15 K and 368 K and Pressure Up to 9 MPa:** | https://www.doi.org/10.1021/acs.jced.5b00134 |
| **Phase equilibria in five binary systems containing 1-butanethiol and 2-methylpropan-2-ol (TBA):** | https://www.doi.org/10.1016/j.fluid.2010.02.030 |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1819 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Liquid-Liquid Equilibria of Ternary Systems Sulfide + Octane + Solvents at Different Temperatures:** | https://www.doi.org/10.1021/je800340v |
| **Measurement through a Gas Stripping Technique of Henry's Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1 = 0.25 and 0.35:** | https://www.doi.org/10.1021/je800349p |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C109795&Units=SI |
| **Infinite dilution activity coefficient measurements by inert gas stripping method:** | https://www.doi.org/10.1016/j.fluid.2006.02.022 |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1819 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Measurement of Henry s Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1 = 0.50 Using a Gas Stripping Technique:** | https://www.doi.org/10.1021/je050268b |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | 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 |
| **nfpaf:** | NFPA Fire Rating |
| **nfpah:** | NFPA Health Rating |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rhoc:** | Critical density |

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |