# 1-Propanethiol, 2,2-dimethyl-

**Other names:** 2,2-Dimethyl-1-propanethiol
2,2-dimethylpropanethiol
Neopentyl mercaptan
**Inchi:** InChI=1S/C5H12S/c1-5(2,3)4-6/h6H,4H2,1-3H3
**InchiKey:** LSUXMVNABVPWMF-UHFFFAOYSA-N
**Formula:** C5H12S
**SMILES:** CC(C)(C)CS
**Mol. weight [g/mol]:** 104.21
**CAS:** 1679-08-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 809.50 | kJ/mol | NIST Webbook |
| basg | 778.20 | kJ/mol | NIST Webbook |
| chl | -4119.40 ± 0.75 | kJ/mol | NIST Webbook |
| gf | 23.45 | kJ/mol | Joback Method |
| hf | -128.70 ± 0.88 | kJ/mol | NIST Webbook |
| hfl | -165.10 ± 0.84 | kJ/mol | NIST Webbook |
| hfus | 5.33 | kJ/mol | Joback Method |
| hvap | 36.40 | kJ/mol | NIST Webbook |
| hvap | 36.40 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 36.80 | kJ/mol | NIST Webbook |
| hvap | 36.40 ± 0.20 | kJ/mol | NIST Webbook |
| log10ws | -1.75 | | Crippen Method |
| logp | 1.962 | | Crippen Method |
| mcvol | 97.660 | ml/mol | McGowan Method |
| pc | 3834.03 | kPa | Joback Method |
| tb | 340.00 ± 10.00 | K | NIST Webbook |
| tb | 340.00 ± 4.00 | K | NIST Webbook |
| tb | 376.85 ± 0.20 | K | NIST Webbook |
| tc | 576.75 | K | Joback Method |
| tf | 184.99 | K | Joback Method |
| vc | 0.358 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 169.61 | J/mol×K | 373.43 | Joback Method |
| cpg | 181.27 | J/mol×K | 407.32 | Joback Method |
| cpg | 192.27 | J/mol×K | 441.20 | Joback Method |
| cpg | 202.63 | J/mol×K | 475.09 | Joback Method |
| cpg | 212.39 | J/mol×K | 508.98 | Joback Method |
| cpg | 221.58 | J/mol×K | 542.86 | Joback Method |
| cpg | 230.22 | J/mol×K | 576.75 | Joback Method |
| hvapt | 36.90 | kJ/mol | 341.50 | NIST Webbook |
| hvapt | 36.20 | kJ/mol | 354.00 | NIST Webbook |
| hvapt | 42.10 | kJ/mol | 314.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.53764e+01 |
| Coeff. B | -3.56030e+03 |
| Coeff. C | -4.59090e+01 |
| Temperature range (K), min. | 281.86 |
| Temperature range (K), max. | 399.64 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679089&Units=SI

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

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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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

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

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |