# 4-Methyl-3-thia-1-pentanethiol

**Inchi:** InChI=1S/C5H12S2/c1-5(2)7-4-3-6/h5-6H,3-4H2,1-2H3
**InchiKey:** VKUMRESRWKKRPX-UHFFFAOYSA-N
**Formula:** C5H12S2
**SMILES:** CC(C)SCCS
**Mol. weight [g/mol]:** 136.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 51.29 | kJ/mol | Joback Method |
| hf | -71.46 | kJ/mol | Joback Method |
| hfus | 13.35 | kJ/mol | Joback Method |
| hvap | 39.89 | kJ/mol | Joback Method |
| log10ws | -1.98 | | Crippen Method |
| logp | 2.058 | | Crippen Method |
| mcvol | 114.010 | ml/mol | McGowan Method |
| pc | 3862.67 | kPa | Joback Method |
| rinpol | 1062.00 | | NIST Webbook |
| rinpol | 1062.00 | | NIST Webbook |
| tb | 445.00 | K | Joback Method |
| tc | 665.67 | K | Joback Method |
| tf | 201.97 | K | Joback Method |
| vc | 0.417 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 212.53 | J/mol×K | 445.00 | Joback Method |
| cpg | 223.80 | J/mol×K | 481.78 | Joback Method |
| cpg | 234.55 | J/mol×K | 518.56 | Joback Method |
| cpg | 244.77 | J/mol×K | 555.33 | Joback Method |
| cpg | 254.47 | J/mol×K | 592.11 | Joback Method |
| cpg | 263.67 | J/mol×K | 628.89 | Joback Method |
| cpg | 272.36 | J/mol×K | 665.67 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R157147&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |