# 4-Mercapto-3-methylpentan-2-ol, # 1

**Inchi:** InChI=1S/C6H14OS/c1-4(5(2)7)6(3)8/h4-8H,1-3H3
**InchiKey:** IAEUQPZVOWVIES-UHFFFAOYSA-N
**Formula:** C6H14OS
**SMILES:** CC(O)C(C)C(C)S
**Mol. weight [g/mol]:** 134.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -115.11 | kJ/mol | Joback Method |
| hf | -296.76 | kJ/mol | Joback Method |
| hfus | 8.86 | kJ/mol | Joback Method |
| hvap | 51.20 | kJ/mol | Joback Method |
| log10ws | -1.65 | | Crippen Method |
| logp | 1.322 | | Crippen Method |
| mcvol | 117.620 | ml/mol | McGowan Method |
| pc | 3838.78 | kPa | Joback Method |
| rinpol | 1022.00 | | NIST Webbook |
| rinpol | 1022.00 | | NIST Webbook |
| tb | 490.40 | K | Joback Method |
| tc | 682.69 | K | Joback Method |
| tf | 209.66 | K | Joback Method |
| vc | 0.426 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 253.69 | J/mol×K | 490.40 | Joback Method |
| cpg | 264.59 | J/mol×K | 522.45 | Joback Method |
| cpg | 274.99 | J/mol×K | 554.50 | Joback Method |
| cpg | 284.88 | J/mol×K | 586.54 | Joback Method |
| cpg | 294.29 | J/mol×K | 618.59 | Joback Method |
| cpg | 303.24 | J/mol×K | 650.64 | Joback Method |
| cpg | 311.73 | J/mol×K | 682.69 | Joback Method |

# Sources

| | |
|---|---|
| **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=R603046&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |