# 1-Mercapto-2-methyl-2-propanol

**Inchi:** InChI=1S/C4H10OS/c1-4(2,5)3-6/h5-6H,3H2,1-2H3
**InchiKey:** FEMWXGBGVVJDFO-UHFFFAOYSA-N
**Formula:** C4H10OS
**SMILES:** CC(C)(O)CS
**Mol. weight [g/mol]:** 106.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -121.79 | kJ/mol | Joback Method |
| hf | -248.39 | kJ/mol | Joback Method |
| hfus | 6.83 | kJ/mol | Joback Method |
| hvap | 46.62 | kJ/mol | Joback Method |
| log10ws | -0.94 | | Crippen Method |
| logp | 0.687 | | Crippen Method |
| mcvol | 89.440 | ml/mol | McGowan Method |
| pc | 4910.80 | kPa | Joback Method |
| rinpol | 954.00 | | NIST Webbook |
| ripol | 1459.00 | | NIST Webbook |
| tb | 442.73 | K | Joback Method |
| tc | 638.63 | K | Joback Method |
| tf | 234.54 | K | Joback Method |
| vc | 0.322 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 176.46 | J/mol×K | 442.73 | Joback Method |
| cpg | 185.11 | J/mol×K | 475.38 | Joback Method |
| cpg | 193.25 | J/mol×K | 508.03 | Joback Method |
| cpg | 200.90 | J/mol×K | 540.68 | Joback Method |
| cpg | 208.08 | J/mol×K | 573.33 | Joback Method |
| cpg | 214.82 | J/mol×K | 605.98 | Joback Method |
| cpg | 221.16 | J/mol×K | 638.63 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R568700&Units=SI |
| **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

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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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |