# cis-4-Methylcyclohexane-1-thiol

**Inchi:** InChI=1S/C7H14S/c1-6-2-4-7(8)5-3-6/h6-8H,2-5H2,1H3/t6-,7+
**InchiKey:** JYGRMXYSBUHFOS-KNVOCYPGSA-N
**Formula:** C7H14S
**SMILES:** CC1CCC(S)CC1
**Mol. weight [g/mol]:** 130.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 54.19 | kJ/mol | Joback Method |
| hf | -115.35 | kJ/mol | Joback Method |
| hfus | 10.83 | kJ/mol | Joback Method |
| hvap | 38.03 | kJ/mol | Joback Method |
| log10ws | -2.59 | | Crippen Method |
| logp | 2.495 | | Crippen Method |
| mcvol | 114.980 | ml/mol | McGowan Method |
| pc | 3655.35 | kPa | Joback Method |
| rinpol | 996.00 | | NIST Webbook |
| tb | 437.30 | K | Joback Method |
| tc | 666.53 | K | Joback Method |
| tf | 208.25 | K | Joback Method |
| vc | 0.413 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 225.46 | J/mol×K | 437.30 | Joback Method |
| cpg | 243.00 | J/mol×K | 475.50 | Joback Method |
| cpg | 259.60 | J/mol×K | 513.71 | Joback Method |
| cpg | 275.28 | J/mol×K | 551.91 | Joback Method |
| cpg | 290.07 | J/mol×K | 590.12 | Joback Method |
| cpg | 303.98 | J/mol×K | 628.32 | Joback Method |
| cpg | 317.03 | J/mol×K | 666.53 | 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=R524304&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 |