# 2-(mercaptomethyl)thiane

**Inchi:** InChI=1S/C6H12S2/c7-5-6-3-1-2-4-8-6/h6-7H,1-5H2
**InchiKey:** YYHUXIOKMLYXRL-UHFFFAOYSA-N
**Formula:** C6H12S2
**SMILES:** SCC1CCCCS1
**Mol. weight [g/mol]:** 148.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 93.34 | kJ/mol | Joback Method |
| hf | -29.11 | kJ/mol | Joback Method |
| hfus | 10.83 | kJ/mol | Joback Method |
| hvap | 41.93 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 2.202 | | Crippen Method |
| mcvol | 117.240 | ml/mol | McGowan Method |
| pc | 4266.28 | kPa | Joback Method |
| rinpol | 1119.00 | | NIST Webbook |
| tb | 466.92 | K | Joback Method |
| tc | 716.52 | K | Joback Method |
| tf | 284.67 | K | Joback Method |
| vc | 0.405 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 228.93 | J/mol×K | 466.92 | Joback Method |
| cpg | 244.88 | J/mol×K | 508.52 | Joback Method |
| cpg | 259.81 | J/mol×K | 550.12 | Joback Method |
| cpg | 273.74 | J/mol×K | 591.72 | Joback Method |
| cpg | 286.73 | J/mol×K | 633.32 | Joback Method |
| cpg | 298.80 | J/mol×K | 674.92 | Joback Method |
| cpg | 309.99 | J/mol×K | 716.52 | 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=R222538&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 |

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