# cis,cis-2,3,5-trimethyl-thiacyclopentane

**Inchi:** InChI=1S/C7H14S/c1-5-4-6(2)8-7(5)3/h5-7H,4H2,1-3H3/t5-,6+,7-/m0/s1
**InchiKey:** MLHOTFJTKPLNPX-XVMARJQXSA-N
**Formula:** C7H14S
**SMILES:** CC1CC(C)C(C)S1
**Mol. weight [g/mol]:** 130.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 69.05 | kJ/mol | Joback Method |
| hf | -122.75 | kJ/mol | Joback Method |
| hfus | 13.62 | kJ/mol | Joback Method |
| hvap | 36.63 | kJ/mol | Joback Method |
| log10ws | -2.51 | | Crippen Method |
| logp | 2.536 | | Crippen Method |
| mcvol | 114.980 | ml/mol | McGowan Method |
| pc | 3149.09 | kPa | Joback Method |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| rinpol | 975.00 | | NIST Webbook |
| tb | 413.33 | K | Joback Method |
| tc | 623.07 | K | Joback Method |
| tf | 254.52 | K | Joback Method |
| vc | 0.412 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 222.18 | J/mol×K | 413.33 | Joback Method |
| cpg | 238.25 | J/mol×K | 448.29 | Joback Method |
| cpg | 253.57 | J/mol×K | 483.24 | Joback Method |
| cpg | 268.15 | J/mol×K | 518.20 | Joback Method |
| cpg | 282.02 | J/mol×K | 553.16 | Joback Method |
| cpg | 295.20 | J/mol×K | 588.11 | Joback Method |
| cpg | 307.68 | J/mol×K | 623.07 | 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=R208889&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 |