# Cyclohexene, 1-methyl-4-[1-methyl-1,2-bis-(methylthio)ethyl]

**Inchi:** InChI=1S/C12H22S2/c1-10-5-7-11(8-6-10)12(2,14-4)9-13-3/h5,11H,6-9H2,1-4H3
**InchiKey:** ITXNNOQCAWZFMP-UHFFFAOYSA-N
**Formula:** C12H22S2
**SMILES:** CSCC(C)(SC)C1CC=C(C)CC1
**Mol. weight [g/mol]:** 230.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 164.02 | kJ/mol | Joback Method |
| hf | -115.39 | kJ/mol | Joback Method |
| hfus | 20.35 | kJ/mol | Joback Method |
| hvap | 56.03 | kJ/mol | Joback Method |
| log10ws | -4.23 | | Crippen Method |
| logp | 4.218 | | Crippen Method |
| mcvol | 197.480 | ml/mol | McGowan Method |
| pc | 2287.14 | kPa | Joback Method |
| rinpol | 1656.00 | | NIST Webbook |
| tb | 631.98 | K | Joback Method |
| tc | 878.41 | K | Joback Method |
| tf | 316.88 | K | Joback Method |
| vc | 0.724 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 509.08 | J/mol×K | 631.98 | Joback Method |
| cpg | 529.56 | J/mol×K | 673.05 | Joback Method |
| cpg | 548.54 | J/mol×K | 714.12 | Joback Method |
| cpg | 566.07 | J/mol×K | 755.19 | Joback Method |
| cpg | 582.22 | J/mol×K | 796.26 | Joback Method |
| cpg | 597.04 | J/mol×K | 837.34 | Joback Method |
| cpg | 610.59 | J/mol×K | 878.41 | Joback Method |

# Sources

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|---|---|
| **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=R121772&Units=SI |

# 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 |