# 3,3-dimethyl-2,4-dithiahexane

**Inchi:** InChI=1S/C6H14S2/c1-5-8-6(2,3)7-4/h5H2,1-4H3
**InchiKey:** FWUMVNGWZBEAIO-UHFFFAOYSA-N
**Formula:** C6H14S2
**SMILES:** CCSC(C)(C)SC
**Mol. weight [g/mol]:** 150.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 68.72 | kJ/mol | Joback Method |
| hf | -92.18 | kJ/mol | Joback Method |
| hfus | 12.14 | kJ/mol | Joback Method |
| hvap | 41.29 | kJ/mol | Joback Method |
| log10ws | -2.71 | | Crippen Method |
| logp | 2.839 | | Crippen Method |
| mcvol | 128.100 | ml/mol | McGowan Method |
| pc | 3299.15 | kPa | Joback Method |
| rinpol | 1046.00 | | NIST Webbook |
| rinpol | 1046.00 | | NIST Webbook |
| tb | 471.01 | K | Joback Method |
| tc | 697.89 | K | Joback Method |
| tf | 228.60 | K | Joback Method |
| vc | 0.469 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 257.06 | J/mol×K | 471.01 | Joback Method |
| cpg | 270.59 | J/mol×K | 508.82 | Joback Method |
| cpg | 283.33 | J/mol×K | 546.64 | Joback Method |
| cpg | 295.30 | J/mol×K | 584.45 | Joback Method |
| cpg | 306.53 | J/mol×K | 622.27 | Joback Method |
| cpg | 317.05 | J/mol×K | 660.08 | Joback Method |
| cpg | 326.87 | J/mol×K | 697.89 | Joback Method |

# Sources

| | |
|---|---|
| **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=R156411&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |