# 1-(4-Methyl-4H-[1,3]dithiin-2-yl)-propane-2-thiol

**Inchi:** InChI=1S/C8H14S3/c1-6(9)5-8-10-4-3-7(2)11-8/h3-4,6-9H,5H2,1-2H3
**InchiKey:** KIZYPBJKLBKTGJ-UHFFFAOYSA-N
**Formula:** C8H14S3
**SMILES:** CC(S)CC1SC=CC(C)S1
**Mol. weight [g/mol]:** 206.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 169.85 | kJ/mol | Joback Method |
| hf | 7.03 | kJ/mol | Joback Method |
| hfus | 18.44 | kJ/mol | Joback Method |
| hvap | 51.79 | kJ/mol | Joback Method |
| log10ws | -4.09 | | Crippen Method |
| logp | 3.403 | | Crippen Method |
| mcvol | 157.470 | ml/mol | McGowan Method |
| pc | 3388.08 | kPa | Joback Method |
| rinpol | 1530.00 | | NIST Webbook |
| tb | 554.56 | K | Joback Method |
| tc | 816.80 | K | Joback Method |
| tf | 372.18 | K | Joback Method |
| vc | 0.541 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 346.42 | J/mol×K | 554.56 | Joback Method |
| cpg | 363.71 | J/mol×K | 598.27 | Joback Method |
| cpg | 379.78 | J/mol×K | 641.97 | Joback Method |
| cpg | 394.67 | J/mol×K | 685.68 | Joback Method |
| cpg | 408.42 | J/mol×K | 729.39 | Joback Method |
| cpg | 421.08 | J/mol×K | 773.09 | Joback Method |
| cpg | 432.69 | J/mol×K | 816.80 | 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=R487275&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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