# 5,5-dimethyl-4-thia-1-heptene

**Other names:** Allyl 1,1-dimethylpropyl sulfide
**Inchi:** InChI=1S/C8H16S/c1-5-7-9-8(3,4)6-2/h5H,1,6-7H2,2-4H3
**InchiKey:** QPQZFYPYIMCHSG-UHFFFAOYSA-N
**Formula:** C8H16S
**SMILES:** C=CCSC(C)(C)CC
**Mol. weight [g/mol]:** 144.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 140.28 | kJ/mol | Joback Method |
| hf | -49.90 | kJ/mol | Joback Method |
| hfus | 11.91 | kJ/mol | Joback Method |
| hvap | 38.25 | kJ/mol | Joback Method |
| log10ws | -3.02 | | Crippen Method |
| logp | 3.094 | | Crippen Method |
| mcvol | 135.630 | ml/mol | McGowan Method |
| pc | 2746.90 | kPa | Joback Method |
| rinpol | 994.00 | | NIST Webbook |
| rinpol | 994.00 | | NIST Webbook |
| tb | 444.67 | K | Joback Method |
| tc | 646.80 | K | Joback Method |
| tf | 214.98 | K | Joback Method |
| vc | 0.507 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 272.88 | J/mol×K | 444.67 | Joback Method |
| cpg | 287.53 | J/mol×K | 478.36 | Joback Method |
| cpg | 301.37 | J/mol×K | 512.05 | Joback Method |
| cpg | 314.44 | J/mol×K | 545.73 | Joback Method |
| cpg | 326.76 | J/mol×K | 579.42 | Joback Method |
| cpg | 338.37 | J/mol×K | 613.11 | Joback Method |
| cpg | 349.30 | J/mol×K | 646.80 | 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=R144042&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 |