# (Z)-1-propenyl sec-butyl disulfide

**Inchi:** InChI=1S/C7H14S2/c1-4-6-8-9-7(3)5-2/h4,6-7H,5H2,1-3H3/b6-4-
**InchiKey:** IOVUOUZQSDBAQN-XQRVVYSFSA-N
**Formula:** C7H14S2
**SMILES:** CC=CSSC(C)CC
**Mol. weight [g/mol]:** 162.32
**CAS:** 24351-70-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 152.08 | kJ/mol | Joback Method |
| hf | 7.87 | kJ/mol | Joback Method |
| hfus | 18.82 | kJ/mol | Joback Method |
| hvap | 44.38 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.700 | | Crippen Method |
| mcvol | 137.890 | ml/mol | McGowan Method |
| pc | 3100.18 | kPa | Joback Method |
| rinpol | 1176.80 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| tb | 500.84 | K | Joback Method |
| tc | 725.26 | K | Joback Method |
| tf | 217.37 | K | Joback Method |
| vc | 0.509 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 279.01 | J/mol×K | 500.84 | Joback Method |
| cpg | 292.38 | J/mol×K | 538.24 | Joback Method |
| cpg | 305.02 | J/mol×K | 575.65 | Joback Method |
| cpg | 316.95 | J/mol×K | 613.05 | Joback Method |
| cpg | 328.19 | J/mol×K | 650.45 | Joback Method |
| cpg | 338.77 | J/mol×K | 687.85 | Joback Method |
| cpg | 348.69 | J/mol×K | 725.26 | 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=C24351700&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 |