# S-Propyl-1-propenethiosulfonate

**Other names:** Propyl 1-propenethiosulfonate, (Z)-
**Inchi:** InChI=1S/C6H12O2S2/c1-3-5-9-10(7,8)6-4-2/h4,6H,3,5H2,1-2H3/b6-4+
**InchiKey:** UBHYKEUMFYXOIJ-GQCTYLIASA-N
**Formula:** C6H12O2S2
**SMILES:** CC=CS(=O)(=O)SCCC
**Mol. weight [g/mol]:** 180.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -355.56 | kJ/mol | Joback Method |
| hf | -461.43 | kJ/mol | Joback Method |
| hfus | 27.01 | kJ/mol | Joback Method |
| hvap | 54.36 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 1.993 | | Crippen Method |
| mcvol | 135.540 | ml/mol | McGowan Method |
| pc | 4056.96 | kPa | Joback Method |
| rinpol | 1381.00 | | NIST Webbook |
| tb | 457.40 | K | Joback Method |
| tc | 651.23 | K | Joback Method |
| tf | 225.26 | K | Joback Method |
| vc | 0.531 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 263.41 | J/mol×K | 457.40 | Joback Method |
| cpg | 275.28 | J/mol×K | 489.71 | Joback Method |
| cpg | 286.62 | J/mol×K | 522.01 | Joback Method |
| cpg | 297.42 | J/mol×K | 554.32 | Joback Method |
| cpg | 307.70 | J/mol×K | 586.62 | Joback Method |
| cpg | 317.45 | J/mol×K | 618.93 | Joback Method |
| cpg | 326.68 | J/mol×K | 651.23 | 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=U322294&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |