# 3-Mercaptoheptanol

**Inchi:** InChI=1S/C7H16OS/c1-2-3-4-7(9)5-6-8/h7-9H,2-6H2,1H3
**InchiKey:** KXCJHOUHCZNWTF-UHFFFAOYSA-N
**Formula:** C7H16OS
**SMILES:** CCCCC(S)CCO
**Mol. weight [g/mol]:** 148.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -101.81 | kJ/mol | Joback Method |
| hf | -306.84 | kJ/mol | Joback Method |
| hfus | 18.49 | kJ/mol | Joback Method |
| hvap | 54.20 | kJ/mol | Joback Method |
| log10ws | -2.20 | | Crippen Method |
| logp | 1.857 | | Crippen Method |
| mcvol | 131.710 | ml/mol | McGowan Method |
| pc | 3356.75 | kPa | Joback Method |
| rinpol | 1286.00 | | NIST Webbook |
| rinpol | 1198.00 | | NIST Webbook |
| rinpol | 1286.00 | | NIST Webbook |
| rinpol | 1198.00 | | NIST Webbook |
| rinpol | 1198.00 | | NIST Webbook |
| ripol | 1956.00 | | NIST Webbook |
| ripol | 1962.00 | | NIST Webbook |
| ripol | 1956.00 | | NIST Webbook |
| ripol | 1962.00 | | NIST Webbook |
| tb | 514.16 | K | Joback Method |
| tc | 696.47 | K | Joback Method |
| tf | 250.93 | K | Joback Method |
| vc | 0.494 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 296.10 | J/mol×K | 514.16 | Joback Method |

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|---|---|---|---|---|
| cpg | 307.40 | J/mol×K | 544.54 | Joback Method |
| cpg | 318.20 | J/mol×K | 574.93 | Joback Method |
| cpg | 328.52 | J/mol×K | 605.31 | Joback Method |
| cpg | 338.36 | J/mol×K | 635.70 | Joback Method |
| cpg | 347.75 | J/mol×K | 666.08 | Joback Method |
| cpg | 356.70 | J/mol×K | 696.47 | 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=R292012&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |