# 5-Methyl-4-mercaptohexan-2-one

**Inchi:** InChI=1S/C7H14OS/c1-5(2)7(9)4-6(3)8/h5,7,9H,4H2,1-3H3
**InchiKey:** UQBDDFZDCXIBHM-UHFFFAOYSA-N
**Formula:** C7H14OS
**SMILES:** CC(=O)CC(S)C(C)C
**Mol. weight [g/mol]:** 146.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -96.35 | kJ/mol | Joback Method |
| hf | -272.47 | kJ/mol | Joback Method |
| hfus | 12.48 | kJ/mol | Joback Method |
| hvap | 43.88 | kJ/mol | Joback Method |
| log10ws | -1.98 | | Crippen Method |
| logp | 1.920 | | Crippen Method |
| mcvol | 127.410 | ml/mol | McGowan Method |
| pc | 3276.53 | kPa | Joback Method |
| rinpol | 1107.00 | | NIST Webbook |
| rinpol | 1069.00 | | NIST Webbook |
| rinpol | 1069.00 | | NIST Webbook |
| rinpol | 1069.00 | | NIST Webbook |
| ripol | 1585.00 | | NIST Webbook |
| ripol | 1585.00 | | NIST Webbook |
| tb | 475.41 | K | Joback Method |
| tc | 682.94 | K | Joback Method |
| tf | 225.04 | K | Joback Method |
| vc | 0.475 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 262.97 | J/mol×K | 475.41 | Joback Method |
| cpg | 275.68 | J/mol×K | 510.00 | Joback Method |
| cpg | 287.76 | J/mol×K | 544.59 | Joback Method |
| cpg | 299.23 | J/mol×K | 579.18 | Joback Method |

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|---|---|---|---|---|
| cpg | 310.10 | J/mol×K | 613.77 | Joback Method |
| cpg | 320.39 | J/mol×K | 648.35 | Joback Method |
| cpg | 330.12 | J/mol×K | 682.94 | 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=R282496&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |