# 2-Propanone, 1-(5-methyl-3H-1,2-dithiol-3-ylidene)-

**Other names:** 3,5-Heptadien-2-one, 4,6-epidithio-
**Inchi:** InChI=1S/C7H8OS2/c1-5(8)3-7-4-6(2)9-10-7/h3-4H,1-2H3/b7-3-
**InchiKey:** YAIGSGPVNPIUNY-CLTKARDFSA-N
**Formula:** C7H8OS2
**SMILES:** CC(=O)C=C1C=C(C)SS1
**Mol. weight [g/mol]:** 172.27
**CAS:** 1005-55-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 68.91 | kJ/mol | Joback Method |
| hf | -6.71 | kJ/mol | Joback Method |
| hfus | 16.82 | kJ/mol | Joback Method |
| hvap | 51.85 | kJ/mol | Joback Method |
| ie | 7.68 | eV | NIST Webbook |
| log10ws | -3.38 | | Crippen Method |
| logp | 2.758 | | Crippen Method |
| mcvol | 124.300 | ml/mol | McGowan Method |
| pc | 4026.13 | kPa | Joback Method |
| tb | 539.82 | K | Joback Method |
| tc | 787.85 | K | Joback Method |
| tf | 424.26 | K | Joback Method |
| vc | 0.436 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 246.89 | J/mol×K | 539.82 | Joback Method |
| cpg | 257.42 | J/mol×K | 581.16 | Joback Method |
| cpg | 267.18 | J/mol×K | 622.50 | Joback Method |
| cpg | 276.24 | J/mol×K | 663.83 | Joback Method |
| cpg | 284.65 | J/mol×K | 705.17 | Joback Method |
| cpg | 292.46 | J/mol×K | 746.51 | Joback Method |
| cpg | 299.72 | J/mol×K | 787.85 | Joback Method |

# Sources

| | |
|---|---|
| **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=C1005556&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |