# 3-(Methylthio)penta-2,4-dione

**Inchi:** InChI=1S/C6H10O2S/c1-4(7)6(9-3)5(2)8/h6H,1-3H3
**InchiKey:** HTVGCUNUQZCFAN-UHFFFAOYSA-N
**Formula:** C6H10O2S
**SMILES:** CSC(C(C)=O)C(C)=O
**Mol. weight [g/mol]:** 146.21
**CAS:** 32113-68-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -227.52 | kJ/mol | Joback Method |
| hf | -355.74 | kJ/mol | Joback Method |
| hfus | 15.10 | kJ/mol | Joback Method |
| hvap | 48.87 | kJ/mol | Joback Method |
| log10ws | -0.89 | | Crippen Method |
| logp | 0.896 | | Crippen Method |
| mcvol | 114.890 | ml/mol | McGowan Method |
| pc | 3704.46 | kPa | Joback Method |
| ripol | 1703.00 | | NIST Webbook |
| ripol | 1703.00 | | NIST Webbook |
| tb | 512.76 | K | Joback Method |
| tc | 728.38 | K | Joback Method |
| tf | 276.64 | K | Joback Method |
| vc | 0.431 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 237.65 | J/mol×K | 512.76 | Joback Method |
| cpg | 247.99 | J/mol×K | 548.70 | Joback Method |
| cpg | 257.80 | J/mol×K | 584.63 | Joback Method |
| cpg | 267.09 | J/mol×K | 620.57 | Joback Method |
| cpg | 275.85 | J/mol×K | 656.50 | Joback Method |
| cpg | 284.10 | J/mol×K | 692.44 | Joback Method |
| cpg | 291.83 | J/mol×K | 728.38 | 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=C32113681&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |