# Thiocyanic acid, 1,1-dimethyl-3-oxobutyl ester

**Inchi:** InChI=1S/C7H11NOS/c1-6(9)4-7(2,3)10-5-8/h4H2,1-3H3
**InchiKey:** KZOYOWHFCLDEAN-UHFFFAOYSA-N
**Formula:** C7H11NOS
**SMILES:** CC(=O)CC(C)(C)SC#N
**Mol. weight [g/mol]:** 157.23
**CAS:** 26094-11-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 48.28 | kJ/mol | Joback Method |
| hf | -102.39 | kJ/mol | Joback Method |
| hfus | 13.71 | kJ/mol | Joback Method |
| hvap | 53.92 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 1.958 | | Crippen Method |
| mcvol | 128.790 | ml/mol | McGowan Method |
| pc | 3032.27 | kPa | Joback Method |
| tb | 581.06 | K | Joback Method |
| tc | 809.82 | K | Joback Method |
| tf | 320.39 | K | Joback Method |
| vc | 0.502 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 291.98 | J/mol×K | 581.06 | Joback Method |
| cpg | 302.59 | J/mol×K | 619.19 | Joback Method |
| cpg | 312.47 | J/mol×K | 657.31 | Joback Method |
| cpg | 321.66 | J/mol×K | 695.44 | Joback Method |
| cpg | 330.18 | J/mol×K | 733.57 | Joback Method |
| cpg | 338.07 | J/mol×K | 771.69 | Joback Method |
| cpg | 345.36 | J/mol×K | 809.82 | 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=C26094111&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |