# 3,4-dihydro-2H-thiopyran-3-one

**Inchi:** InChI=1S/C5H6OS/c7-5-2-1-3-6-4-5/h1,3H,2,4H2
**InchiKey:** FUTCFJQVPUDGAC-UHFFFAOYSA-N
**Formula:** C5H6OS
**SMILES:** S=C1CC=COC1
**Mol. weight [g/mol]:** 114.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 58.07 | kJ/mol | Joback Method |
| hf | -30.99 | kJ/mol | Joback Method |
| hfus | 14.71 | kJ/mol | Joback Method |
| hvap | 39.74 | kJ/mol | Joback Method |
| log10ws | -1.60 | | Crippen Method |
| logp | 1.290 | | Crippen Method |
| mcvol | 84.070 | ml/mol | McGowan Method |
| pc | 5335.72 | kPa | Joback Method |
| rinpol | 1155.00 | | NIST Webbook |
| tb | 436.77 | K | Joback Method |
| tc | 673.38 | K | Joback Method |
| tf | 248.73 | K | Joback Method |
| vc | 0.294 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 147.37 | J/mol×K | 436.77 | Joback Method |
| cpg | 157.36 | J/mol×K | 476.20 | Joback Method |
| cpg | 166.57 | J/mol×K | 515.64 | Joback Method |
| cpg | 175.04 | J/mol×K | 555.07 | Joback Method |
| cpg | 182.84 | J/mol×K | 594.51 | Joback Method |
| cpg | 190.00 | J/mol×K | 633.94 | Joback Method |
| cpg | 196.59 | J/mol×K | 673.38 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R223833&Units=SI |
| **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 |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |