# 3-ethyl-1,2-dithiolan-4-one

**Other names:** 1,2-Dithiolan-4-one, 3-ethyl
**Inchi:** InChI=1S/C5H8OS2/c1-2-5-4(6)3-7-8-5/h5H,2-3H2,1H3
**InchiKey:** TUMVOBRANVUYMK-UHFFFAOYSA-N
**Formula:** C5H8OS2
**SMILES:** CCC1SSCC1=O
**Mol. weight [g/mol]:** 148.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -15.10 | kJ/mol | Joback Method |
| hf | -133.23 | kJ/mol | Joback Method |
| hfus | 9.46 | kJ/mol | Joback Method |
| hvap | 42.85 | kJ/mol | Joback Method |
| log10ws | -1.96 | | Crippen Method |
| logp | 1.729 | | Crippen Method |
| mcvol | 104.720 | ml/mol | McGowan Method |
| pc | 4474.22 | kPa | Joback Method |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1167.00 | | NIST Webbook |
| rinpol | 1163.00 | | NIST Webbook |
| tb | 492.56 | K | Joback Method |
| tc | 745.51 | K | Joback Method |
| tf | 392.13 | K | Joback Method |
| vc | 0.355 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 208.04 | J/mol×K | 492.56 | Joback Method |
| cpg | 220.32 | J/mol×K | 534.72 | Joback Method |
| cpg | 231.96 | J/mol×K | 576.88 | Joback Method |
| cpg | 242.96 | J/mol×K | 619.03 | Joback Method |
| cpg | 253.30 | J/mol×K | 661.19 | Joback Method |
| cpg | 262.99 | J/mol×K | 703.35 | Joback Method |

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|---|---|---|---|---|
| cpg | 272.02 | J/mol×K | 745.51 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R90363&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 |