# 2-oxopropyl 2-oxo-3-pentyl disulfide

**Inchi:** InChI=1S/C8H14O2S2/c1-4-8(7(3)10)12-11-5-6(2)9/h8H,4-5H2,1-3H3
**InchiKey:** JZQCBSPQQKJGDF-UHFFFAOYSA-N
**Formula:** C8H14O2S2
**SMILES:** CCC(SSCC(C)=O)C(C)=O
**Mol. weight [g/mol]:** 206.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -177.56 | kJ/mol | Joback Method |
| hf | -355.15 | kJ/mol | Joback Method |
| hfus | 24.41 | kJ/mol | Joback Method |
| hvap | 60.14 | kJ/mol | Joback Method |
| log10ws | -2.60 | | Crippen Method |
| logp | 2.324 | | Crippen Method |
| mcvol | 159.420 | ml/mol | McGowan Method |
| pc | 3025.61 | kPa | Joback Method |
| rinpol | 1506.00 | | NIST Webbook |
| rinpol | 1506.00 | | NIST Webbook |
| ripol | 2308.00 | | NIST Webbook |
| tb | 627.30 | K | Joback Method |
| tc | 853.59 | K | Joback Method |
| tf | 333.58 | K | Joback Method |
| vc | 0.598 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 374.29 | J/mol×K | 627.30 | Joback Method |
| cpg | 386.80 | J/mol×K | 665.02 | Joback Method |
| cpg | 398.53 | J/mol×K | 702.73 | Joback Method |
| cpg | 409.47 | J/mol×K | 740.45 | Joback Method |
| cpg | 419.63 | J/mol×K | 778.16 | Joback Method |
| cpg | 429.02 | J/mol×K | 815.88 | Joback Method |
| cpg | 437.64 | J/mol×K | 853.59 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R224118&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 |

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