# trans-2-(mercaptomethyl)-4-methyl-1,3-dioxolane

**Inchi:** InChI=1S/C5H10O2S/c1-4-2-6-5(3-8)7-4/h4-5,8H,2-3H2,1H3/t4-,5-/m0/s1
**InchiKey:** IZIJAPPJBKUSNQ-WHFBIAKZSA-N
**Formula:** C5H10O2S
**SMILES:** CC1COC(CS)O1
**Mol. weight [g/mol]:** 134.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -122.79 | kJ/mol | Joback Method |
| hf | -331.91 | kJ/mol | Joback Method |
| hfus | 23.71 | kJ/mol | Joback Method |
| hvap | 42.43 | kJ/mol | Joback Method |
| log10ws | -0.78 | | Crippen Method |
| logp | 0.678 | | Crippen Method |
| mcvol | 98.540 | ml/mol | McGowan Method |
| pc | 4414.96 | kPa | Joback Method |
| rinpol | 959.00 | | NIST Webbook |
| ripol | 1476.00 | | NIST Webbook |
| tb | 441.17 | K | Joback Method |
| tc | 665.59 | K | Joback Method |
| tf | 242.37 | K | Joback Method |
| vc | 0.351 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 203.21 | J/mol×K | 441.17 | Joback Method |
| cpg | 216.16 | J/mol×K | 478.57 | Joback Method |
| cpg | 228.42 | J/mol×K | 515.98 | Joback Method |
| cpg | 240.00 | J/mol×K | 553.38 | Joback Method |
| cpg | 250.93 | J/mol×K | 590.78 | Joback Method |
| cpg | 261.21 | J/mol×K | 628.18 | Joback Method |
| cpg | 270.86 | J/mol×K | 665.59 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R169318&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 |