# 1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-

**Other names:** 2-tert-Butyl-5-methyl-1,3-dioxan-4-one
**Inchi:** InChI=1S/C9H16O3/c1-6-5-11-8(9(2,3)4)12-7(6)10/h6,8H,5H2,1-4H3/t6-,8+/m1/s1
**InchiKey:** IDAKACQLSWKCND-SVRRBLITSA-N
**Formula:** C9H16O3
**SMILES:** CC1COC(C(C)(C)C)OC1=O
**Mol. weight [g/mol]:** 172.22
**CAS:** 107289-32-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -250.35 | kJ/mol | Joback Method |
| hf | -605.56 | kJ/mol | Joback Method |
| hfus | 20.03 | kJ/mol | Joback Method |
| hvap | 47.72 | kJ/mol | Joback Method |
| log10ws | -1.56 | | Crippen Method |
| logp | 1.568 | | Crippen Method |
| mcvol | 140.120 | ml/mol | McGowan Method |
| pc | 2847.48 | kPa | Joback Method |
| rinpol | 1251.00 | | NIST Webbook |
| rinpol | 1251.00 | | NIST Webbook |
| tb | 538.69 | K | Joback Method |
| tc | 766.01 | K | Joback Method |
| tf | 318.11 | K | Joback Method |
| vc | 0.509 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 359.04 | J/mol×K | 538.69 | Joback Method |
| cpg | 377.49 | J/mol×K | 576.58 | Joback Method |
| cpg | 394.91 | J/mol×K | 614.46 | Joback Method |
| cpg | 411.31 | J/mol×K | 652.35 | Joback Method |
| cpg | 426.69 | J/mol×K | 690.24 | Joback Method |
| cpg | 441.06 | J/mol×K | 728.13 | Joback Method |

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|---|---|---|---|---|
| cpg | 454.42 | J/mol×K | 766.01 | Joback Method |

# Sources

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|---|---|
| **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=C107289327&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |