# 5,5-Dimethyl-2-isopropyl-1,3-dioxane

**Other names:** 2-Isopropyl-5,5-Dimethyl-1,3-dioxane
**Inchi:** InChI=1S/C9H18O2/c1-7(2)8-10-5-9(3,4)6-11-8/h7-8H,5-6H2,1-4H3
**InchiKey:** AWSZUOKHFRWQFK-UHFFFAOYSA-N
**Formula:** C9H18O2
**SMILES:** CC(C)C1OCC(C)(C)CO1
**Mol. weight [g/mol]:** 158.24
**CAS:** 7651-50-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -138.53 | kJ/mol | Joback Method |
| hf | -449.15 | kJ/mol | Joback Method |
| hfus | 18.11 | kJ/mol | Joback Method |
| hvap | 43.23 | kJ/mol | Joback Method |
| log10ws | -1.78 | | Crippen Method |
| logp | 2.042 | | Crippen Method |
| mcvol | 138.550 | ml/mol | McGowan Method |
| pc | 2844.44 | kPa | Joback Method |
| tb | 473.90 | K | Joback Method |
| tc | 685.12 | K | Joback Method |
| tf | 256.37 | K | Joback Method |
| vc | 0.505 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 322.21 | J/mol×K | 473.90 | Joback Method |
| cpg | 340.62 | J/mol×K | 509.10 | Joback Method |
| cpg | 357.91 | J/mol×K | 544.31 | Joback Method |
| cpg | 374.17 | J/mol×K | 579.51 | Joback Method |
| cpg | 389.49 | J/mol×K | 614.71 | Joback Method |
| cpg | 403.96 | J/mol×K | 649.92 | Joback Method |
| cpg | 417.69 | J/mol×K | 685.12 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7651505&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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