# 1,4-Dioxyl radical

**Inchi:** InChI=1S/C4H7O2/c1-2-6-4-3-5-1/h1H,2-4H2
**InchiKey:** XTKIUJCPLLOSMW-UHFFFAOYSA-N
**Formula:** C4H7O2
**SMILES:** [CH]1COCCO1
**Mol. weight [g/mol]:** 87.10
**CAS:** 4598-47-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 803.20 | kJ/mol | NIST Webbook |
| basg | 770.70 | kJ/mol | NIST Webbook |
| gf | -112.61 | kJ/mol | Joback Method |
| hf | -279.76 | kJ/mol | Joback Method |
| hfus | 15.59 | kJ/mol | Joback Method |
| hvap | 33.80 | kJ/mol | Joback Method |
| log10ws | 0.33 | | Crippen Method |
| logp | 0.195 | | Crippen Method |
| mcvol | 65.950 | ml/mol | McGowan Method |
| pc | 5320.16 | kPa | Joback Method |
| tb | 363.67 | K | Joback Method |
| tc | 568.40 | K | Joback Method |
| tf | 211.73 | K | Joback Method |
| vc | 0.226 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 113.67 | J/mol×K | 363.67 | Joback Method |
| cpg | 124.48 | J/mol×K | 397.79 | Joback Method |
| cpg | 134.61 | J/mol×K | 431.91 | Joback Method |
| cpg | 144.10 | J/mol×K | 466.03 | Joback Method |
| cpg | 152.97 | J/mol×K | 500.15 | Joback Method |
| cpg | 161.26 | J/mol×K | 534.28 | Joback Method |
| cpg | 169.01 | J/mol×K | 568.40 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0025959 | Pa×s | 211.73 | Joback Method |
| dvisc | 0.0017242 | Pa×s | 237.05 | Joback Method |
| dvisc | 0.0012394 | Pa×s | 262.38 | Joback Method |
| dvisc | 0.0009442 | Pa×s | 287.70 | Joback Method |
| dvisc | 0.0007517 | Pa×s | 313.02 | Joback Method |
| dvisc | 0.0006192 | Pa×s | 338.35 | Joback Method |
| dvisc | 0.0005240 | Pa×s | 363.67 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4598474&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

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |

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