# 1,3-Dioxane

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|---|---|
| **Other names:** | 1,3-Dioxacyclohexane |
| | 1,3-Propanediol formal |
| | m-Dioxane |
| | m-Dioxin, dihydro- |
| **Inchi:** | InChI=1S/C4H8O2/c1-2-5-4-6-3-1/h1-4H2 |
| **InchiKey:** | VDFVNEFVBPFDSB-UHFFFAOYSA-N |
| **Formula:** | C4H8O2 |
| **SMILES:** | C1COCOC1 |
| **Mol. weight [g/mol]:** | 88.11 |
| **CAS:** | 505-22-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 825.40 | kJ/mol | NIST Webbook |
| basg | 796.20 | kJ/mol | NIST Webbook |
| gf | -157.28 | kJ/mol | Joback Method |
| hf | -338.40 ± 1.10 | kJ/mol | NIST Webbook |
| hf | -349.60 | kJ/mol | NIST Webbook |
| hf | -350.00 ± 2.00 | kJ/mol | NIST Webbook |
| hf | -341.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfl | -385.00 ± 1.00 | kJ/mol | NIST Webbook |
| hfl | -377.50 ± 1.10 | kJ/mol | NIST Webbook |
| hfl | -384.60 ± 1.80 | kJ/mol | NIST Webbook |
| hfl | -376.60 ± 0.84 | kJ/mol | NIST Webbook |
| hfus | 12.84 | kJ/mol | Joback Method |
| hvap | 36.00 ± 0.80 | kJ/mol | NIST Webbook |
| hvap | 39.09 ± 0.05 | kJ/mol | NIST Webbook |
| hvap | 35.60 | kJ/mol | NIST Webbook |
| hvap | 39.10 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 35.00 | kJ/mol | NIST Webbook |
| hvap | 39.10 | kJ/mol | NIST Webbook |
| ie | 10.33 | eV | NIST Webbook |
| ie | 10.10 | eV | NIST Webbook |
| ie | 10.12 | eV | NIST Webbook |
| ie | 10.12 | eV | NIST Webbook |
| log10ws | -0.06 | | Crippen Method |
| logp | 0.381 | | Crippen Method |

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|---|---|---|---|
| mcvol | 68.100 | ml/mol | McGowan Method |
| pc | 5235.81 | kPa | Joback Method |
| rinpol | 707.00 | | NIST Webbook |
| rinpol | 720.00 | | NIST Webbook |
| rinpol | 701.00 | | NIST Webbook |
| tb | 378.70 | K | NIST Webbook |
| tc | 578.47 | K | Joback Method |
| tf | 199.60 | K | Joback Method |
| vc | 0.235 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 176.66 | J/mol×K | 578.47 | Joback Method |
| cpg | 168.26 | J/mol×K | 543.56 | Joback Method |
| cpg | 159.34 | J/mol×K | 508.66 | Joback Method |
| cpg | 149.90 | J/mol×K | 473.75 | Joback Method |
| cpg | 139.92 | J/mol×K | 438.85 | Joback Method |
| cpg | 129.39 | J/mol×K | 403.94 | Joback Method |
| cpg | 118.28 | J/mol×K | 369.04 | Joback Method |
| cpl | 143.90 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0004429 | Pa×s | 369.04 | Joback Method |
| dvisc | 0.0006220 | Pa×s | 340.80 | Joback Method |
| dvisc | 0.0009289 | Pa×s | 312.56 | Joback Method |
| dvisc | 0.0015023 | Pa×s | 284.32 | Joback Method |
| dvisc | 0.0027013 | Pa×s | 256.08 | Joback Method |
| dvisc | 0.0056179 | Pa×s | 227.84 | Joback Method |
| dvisc | 0.0143730 | Pa×s | 199.60 | Joback Method |
| hvapt | 39.00 | kJ/mol | 293.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 378.20 | K | 101.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52109e+01 |
| Coeff. B | -3.82420e+03 |
| Coeff. C | -1.76730e+01 |
| Temperature range (K), min. | 273.93 |
| Temperature range (K), max. | 403.98 |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 298.2 K:** | https://www.doi.org/10.1021/je900711h |
| **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=C505226&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |

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|---|---|
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |