# Cyclohexane, 1,1-dimethoxy-

**Other names:** Cyclohexanone, dimethyl acetal
Cyclohexanone dimethyl ketal
1,1-Dimethoxycyclohexane
**Inchi:** InChI=1S/C8H16O2/c1-9-8(10-2)6-4-3-5-7-8/h3-7H2,1-2H3
**InchiKey:** XPIJMQVLTXAGME-UHFFFAOYSA-N
**Formula:** C8H16O2
**SMILES:** COC1(OC)CCCCC1
**Mol. weight [g/mol]:** 144.21
**CAS:** 933-40-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -174.56 | kJ/mol | Joback Method |
| hf | -441.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfl | -492.00 ± 0.80 | kJ/mol | NIST Webbook |
| hfus | 4.39 | kJ/mol | Joback Method |
| hvap | 51.00 | kJ/mol | NIST Webbook |
| hvap | 48.60 ± 0.20 | kJ/mol | NIST Webbook |
| ie | 9.00 | eV | NIST Webbook |
| ie | 9.52 | eV | NIST Webbook |
| log10ws | -1.85 | | Crippen Method |
| logp | 1.940 | | Crippen Method |
| mcvol | 124.460 | ml/mol | McGowan Method |
| pc | 3191.93 | kPa | Joback Method |
| tb | 447.07 | K | Joback Method |
| tc | 655.06 | K | Joback Method |
| tf | 255.66 | K | Joback Method |
| vc | 0.451 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 265.79 | J/mol×K | 447.07 | Joback Method |
| cpg | 282.71 | J/mol×K | 481.74 | Joback Method |

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|---|---|---|---|---|
| cpg | 298.68 | J/mol×K | 516.40 | Joback Method |
| cpg | 313.77 | J/mol×K | 551.07 | Joback Method |
| cpg | 328.06 | J/mol×K | 585.73 | Joback Method |
| cpg | 341.60 | J/mol×K | 620.40 | Joback Method |
| cpg | 354.47 | J/mol×K | 655.06 | Joback Method |
| hvapt | 49.00 ± 0.20 | kJ/mol | 293.00 | NIST Webbook |
| hvapt | 52.40 | kJ/mol | 331.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 328.00 ± 1.00 | K | 1.70 | NIST Webbook |

# 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=C933404&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
**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
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure

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