# Cyclohexanecarboxylic acid, 1-propyl-, methyl ester

**Other names:** Methyl 1-propyl-1-cyclohexanecarboxylate
**Inchi:** InChI=1S/C11H20O2/c1-3-7-11(10(12)13-2)8-5-4-6-9-11/h3-9H2,1-2H3
**InchiKey:** KWFNANKQDJOTPK-UHFFFAOYSA-N
**Formula:** C11H20O2
**SMILES:** CCCC1(C(=O)OC)CCCCC1
**Mol. weight [g/mol]:** 184.28
**CAS:** 4630-86-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -173.22 | kJ/mol | Joback Method |
| hf | -445.61 | kJ/mol | Joback Method |
| hfus | 12.57 | kJ/mol | Joback Method |
| hvap | 48.51 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.910 | | Crippen Method |
| mcvol | 162.430 | ml/mol | McGowan Method |
| pc | 2555.92 | kPa | Joback Method |
| rinpol | 1200.00 | | NIST Webbook |
| rinpol | 1200.00 | | NIST Webbook |
| tb | 547.16 | K | Joback Method |
| tc | 757.58 | K | Joback Method |
| tf | 317.17 | K | Joback Method |
| vc | 0.607 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 403.30 | J/mol×K | 547.16 | Joback Method |
| cpg | 421.68 | J/mol×K | 582.23 | Joback Method |
| cpg | 439.01 | J/mol×K | 617.30 | Joback Method |
| cpg | 455.40 | J/mol×K | 652.37 | Joback Method |
| cpg | 470.93 | J/mol×K | 687.44 | Joback Method |
| cpg | 485.70 | J/mol×K | 722.51 | Joback Method |

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|---|---|---|---|---|
| cpg | 499.81 | J/mol×K | 757.58 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4630868&Units=SI |

# 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 |