# 1,2-Cyclohexanedicarboxylic acid, methyl pentyl ester

**Inchi:** InChI=1S/C14H24O4/c1-3-4-7-10-18-14(16)12-9-6-5-8-11(12)13(15)17-2/h11-12H,3-10H

**InchiKey:** GOYMMNONSQVAHI-UHFFFAOYSA-N

**Formula:** C14H24O4

**SMILES:** CCCCCOC(=O)C1CCCCC1C(=O)OC

**Mol. weight [g/mol]:** 256.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -384.10 | kJ/mol | Joback Method |
| hf | -787.91 | kJ/mol | Joback Method |
| hfus | 30.50 | kJ/mol | Joback Method |
| hvap | 65.19 | kJ/mol | Joback Method |
| log10ws | -2.82 | | Crippen Method |
| logp | 2.699 | | Crippen Method |
| mcvol | 212.140 | ml/mol | McGowan Method |
| pc | 1893.65 | kPa | Joback Method |
| rinpol | 1776.00 | | NIST Webbook |
| rinpol | 1776.00 | | NIST Webbook |
| tb | 687.18 | K | Joback Method |
| tc | 886.79 | K | Joback Method |
| tf | 395.00 | K | Joback Method |
| vc | 0.799 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 618.12 | J/mol×K | 687.18 | Joback Method |
| cpg | 636.45 | J/mol×K | 720.45 | Joback Method |
| cpg | 653.72 | J/mol×K | 753.72 | Joback Method |
| cpg | 669.91 | J/mol×K | 786.99 | Joback Method |
| cpg | 685.04 | J/mol×K | 820.26 | Joback Method |
| cpg | 699.10 | J/mol×K | 853.52 | Joback Method |
| cpg | 712.09 | J/mol×K | 886.79 | Joback Method |
| dvisc | 0.0017019 | Pa×s | 395.00 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0009129 | Pa×s | 443.70 | Joback Method |
| dvisc | 0.0005539 | Pa×s | 492.39 | Joback Method |
| dvisc | 0.0003677 | Pa×s | 541.09 | Joback Method |
| dvisc | 0.0002611 | Pa×s | 589.79 | Joback Method |
| dvisc | 0.0001954 | Pa×s | 638.48 | Joback Method |
| dvisc | 0.0001524 | Pa×s | 687.18 | Joback Method |

# Sources

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|---|---|
| **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=U339652&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |