# 1,2-Cyclohexanedicarboxylic acid, allyl ethyl ester

**Inchi:** InChI=1S/C13H20O4/c1-3-9-17-13(15)11-8-6-5-7-10(11)12(14)16-4-2/h3,10-11H,1,4-9H2

**InchiKey:** ZBIHKDSKBYSVLG-UHFFFAOYSA-N

**Formula:** C13H20O4

**SMILES:** C=CCOC(=O)C1CCCCC1C(=O)OCC

**Mol. weight [g/mol]:** 240.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -304.68 | kJ/mol | Joback Method |
| hf | -641.84 | kJ/mol | Joback Method |
| hfus | 26.63 | kJ/mol | Joback Method |
| hvap | 62.29 | kJ/mol | Joback Method |
| log10ws | -2.25 | | Crippen Method |
| logp | 2.085 | | Crippen Method |
| mcvol | 193.750 | ml/mol | McGowan Method |
| pc | 2143.35 | kPa | Joback Method |
| rinpol | 1630.00 | | NIST Webbook |
| rinpol | 1630.00 | | NIST Webbook |
| tb | 660.98 | K | Joback Method |
| tc | 866.52 | K | Joback Method |
| tf | 381.97 | K | Joback Method |
| vc | 0.725 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 540.16 | J/mol×K | 660.98 | Joback Method |
| cpg | 617.42 | J/mol×K | 832.27 | Joback Method |
| cpg | 604.03 | J/mol×K | 798.01 | Joback Method |
| cpg | 589.61 | J/mol×K | 763.75 | Joback Method |
| cpg | 574.16 | J/mol×K | 729.49 | Joback Method |
| cpg | 557.68 | J/mol×K | 695.24 | Joback Method |
| cpg | 629.78 | J/mol×K | 866.52 | Joback Method |
| dvisc | 0.0001788 | Pa×s | 660.98 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002269 | Pa×s | 614.48 | Joback Method |
| dvisc | 0.0002994 | Pa×s | 567.98 | Joback Method |
| dvisc | 0.0004152 | Pa×s | 521.48 | Joback Method |
| dvisc | 0.0006139 | Pa×s | 474.97 | Joback Method |
| dvisc | 0.0009880 | Pa×s | 428.47 | Joback Method |
| dvisc | 0.0017854 | Pa×s | 381.97 | 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=U339478&Units=SI |

# 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 |