# 1,2-Cyclohexanedicarboxylic acid, allyl pentyl ester

**Inchi:** InChI=1S/C16H26O4/c1-3-5-8-12-20-16(18)14-10-7-6-9-13(14)15(17)19-11-4-2/h4,13-14

**InchiKey:** PTICFFHNHCPTAL-UHFFFAOYSA-N

**Formula:** C16H26O4

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

**Mol. weight [g/mol]:** 282.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -279.42 | kJ/mol | Joback Method |
| hf | -703.76 | kJ/mol | Joback Method |
| hfus | 34.40 | kJ/mol | Joback Method |
| hvap | 68.97 | kJ/mol | Joback Method |
| log10ws | -3.51 | | Crippen Method |
| logp | 3.255 | | Crippen Method |
| mcvol | 236.020 | ml/mol | McGowan Method |
| pc | 1668.70 | kPa | Joback Method |
| rinpol | 1917.00 | | NIST Webbook |
| rinpol | 1917.00 | | NIST Webbook |
| tb | 729.62 | K | Joback Method |
| tc | 928.35 | K | Joback Method |
| tf | 415.78 | K | Joback Method |
| vc | 0.892 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 706.42 | J/mol×K | 729.62 | Joback Method |
| cpg | 724.72 | J/mol×K | 762.74 | Joback Method |
| cpg | 741.87 | J/mol×K | 795.86 | Joback Method |
| cpg | 757.90 | J/mol×K | 828.98 | Joback Method |
| cpg | 772.80 | J/mol×K | 862.10 | Joback Method |
| cpg | 786.59 | J/mol×K | 895.22 | Joback Method |
| cpg | 799.29 | J/mol×K | 928.35 | Joback Method |
| dvisc | 0.0014624 | Pa×s | 415.78 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0007745 | Pa×s | 468.09 | Joback Method |
| dvisc | 0.0004661 | Pa×s | 520.39 | Joback Method |
| dvisc | 0.0003078 | Pa×s | 572.70 | Joback Method |
| dvisc | 0.0002178 | Pa×s | 625.01 | Joback Method |
| dvisc | 0.0001626 | Pa×s | 677.31 | Joback Method |
| dvisc | 0.0001266 | Pa×s | 729.62 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U339482&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |