# 1,2-Cyclohexanedicarboxylic acid, 2-chloroethyl ethyl ester

**Inchi:** InChI=1S/C12H19ClO4/c1-2-16-11(14)9-5-3-4-6-10(9)12(15)17-8-7-13/h9-10H,2-8H2,1H

**InchiKey:** RARRJWGBOLTBKO-UHFFFAOYSA-N

**Formula:** C12H19ClO4

**SMILES:** CCOC(=O)C1CCCCC1C(=O)OCCCl

**Mol. weight [g/mol]:** 262.73

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -412.87 | kJ/mol | Joback Method |
| hf | -762.37 | kJ/mol | Joback Method |
| hfus | 29.51 | kJ/mol | Joback Method |
| hvap | 65.12 | kJ/mol | Joback Method |
| log10ws | -2.14 | | Crippen Method |
| logp | 2.138 | | Crippen Method |
| mcvol | 196.200 | ml/mol | McGowan Method |
| pc | 2177.49 | kPa | Joback Method |
| rinpol | 1770.00 | | NIST Webbook |
| tb | 678.85 | K | Joback Method |
| tc | 887.17 | K | Joback Method |
| tf | 402.38 | K | Joback Method |
| vc | 0.737 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 539.80 | J/mol×K | 678.85 | Joback Method |
| cpg | 556.35 | J/mol×K | 713.57 | Joback Method |
| cpg | 571.88 | J/mol×K | 748.29 | Joback Method |
| cpg | 586.37 | J/mol×K | 783.01 | Joback Method |
| cpg | 599.83 | J/mol×K | 817.73 | Joback Method |
| cpg | 612.25 | J/mol×K | 852.45 | Joback Method |
| cpg | 623.64 | J/mol×K | 887.17 | Joback Method |
| dvisc | 0.0016720 | Pa×s | 402.38 | Joback Method |
| dvisc | 0.0009474 | Pa×s | 448.46 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005967 | Pa×s | 494.54 | Joback Method |
| dvisc | 0.0004067 | Pa×s | 540.62 | Joback Method |
| dvisc | 0.0002944 | Pa×s | 586.69 | Joback Method |
| dvisc | 0.0002233 | Pa×s | 632.77 | Joback Method |
| dvisc | 0.0001759 | Pa×s | 678.85 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U340040&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

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