# 1,2-Cyclohexanedicarboxylic acid, 2-ethoxyethyl pentadecyl ester

**Inchi:** InChI=1S/C27H50O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-18-21-31-26(28)24-19-16-17-20

**InchiKey:** ICYRTSYWYSTSJB-UHFFFAOYSA-N

**Formula:** C27H50O5

**SMILES:** CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC

**Mol. weight [g/mol]:** 454.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -379.64 | kJ/mol | Joback Method |
| hf | -1188.45 | kJ/mol | Joback Method |
| hfus | 65.35 | kJ/mol | Joback Method |
| hvap | 96.54 | kJ/mol | Joback Method |
| log10ws | -7.35 | | Crippen Method |
| logp | 7.007 | | Crippen Method |
| mcvol | 401.180 | ml/mol | McGowan Method |
| pc | 787.71 | kPa | Joback Method |
| rinpol | 3116.00 | | NIST Webbook |
| rinpol | 3116.00 | | NIST Webbook |
| tb | 1007.04 | K | Joback Method |
| tc | 1237.96 | K | Joback Method |
| tf | 563.74 | K | Joback Method |
| vc | 1.546 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1441.36 | J/mol×K | 1007.04 | Joback Method |
| cpg | 1460.80 | J/mol×K | 1045.53 | Joback Method |
| cpg | 1477.99 | J/mol×K | 1084.01 | Joback Method |
| cpg | 1492.98 | J/mol×K | 1122.50 | Joback Method |
| cpg | 1505.79 | J/mol×K | 1160.99 | Joback Method |
| cpg | 1516.47 | J/mol×K | 1199.48 | Joback Method |
| cpg | 1525.05 | J/mol×K | 1237.96 | Joback Method |
| dvisc | 0.0003076 | Pa×s | 563.74 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001471 | Pa×s | 637.62 | Joback Method |
| dvisc | 0.0000820 | Pa×s | 711.51 | Joback Method |
| dvisc | 0.0000510 | Pa×s | 785.39 | Joback Method |
| dvisc | 0.0000345 | Pa×s | 859.27 | Joback Method |
| dvisc | 0.0000248 | Pa×s | 933.16 | Joback Method |
| dvisc | 0.0000187 | Pa×s | 1007.04 | 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=U339916&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 |