# 1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl undecyl ester

**Inchi:** InChI=1S/C27H48O4/c1-2-3-4-5-6-7-8-9-15-21-30-26(28)24-18-13-14-19-25(24)27(29)31

**InchiKey:** GNSJGDZFWNZPSG-UHFFFAOYSA-N

**Formula:** C27H48O4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

**Mol. weight [g/mol]:** 436.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -250.19 | kJ/mol | Joback Method |
| hf | -1001.91 | kJ/mol | Joback Method |
| hfus | 56.00 | kJ/mol | Joback Method |
| hvap | 94.56 | kJ/mol | Joback Method |
| log10ws | -7.91 | | Crippen Method |
| logp | 7.380 | | Crippen Method |
| mcvol | 384.450 | ml/mol | McGowan Method |
| pc | 895.87 | kPa | Joback Method |
| rinpol | 3129.00 | | NIST Webbook |
| rinpol | 3129.00 | | NIST Webbook |
| tb | 1004.17 | K | Joback Method |
| tc | 1229.43 | K | Joback Method |
| tf | 548.89 | K | Joback Method |
| vc | 1.460 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1406.37 | J/mol×K | 1004.17 | Joback Method |
| cpg | 1480.55 | J/mol×K | 1191.89 | Joback Method |
| cpg | 1469.72 | J/mol×K | 1154.34 | Joback Method |
| cpg | 1456.95 | J/mol×K | 1116.80 | Joback Method |
| cpg | 1442.17 | J/mol×K | 1079.26 | Joback Method |
| cpg | 1425.33 | J/mol×K | 1041.71 | Joback Method |
| cpg | 1489.48 | J/mol×K | 1229.43 | Joback Method |
| dvisc | 0.0000260 | Pa×s | 1004.17 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000349 | Pa×s | 928.29 | Joback Method |
| dvisc | 0.0000492 | Pa×s | 852.41 | Joback Method |
| dvisc | 0.0000743 | Pa×s | 776.53 | Joback Method |
| dvisc | 0.0001226 | Pa×s | 700.65 | Joback Method |
| dvisc | 0.0002284 | Pa×s | 624.77 | Joback Method |
| dvisc | 0.0005055 | Pa×s | 548.89 | Joback Method |

# Sources

| | |
|---|---|
| **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=U339731&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 |

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