# 1,2-Cyclohexanedicarboxylic acid, 4-octyl undecyl ester

**Inchi:** InChI=1S/C27H50O4/c1-4-7-9-10-11-12-13-14-17-22-30-26(28)24-20-15-16-21-25(24)27

**InchiKey:** HWWRYSLWCDJQBG-UHFFFAOYSA-N

**Formula:** C27H50O4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC

**Mol. weight [g/mol]:** 438.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -277.08 | kJ/mol | Joback Method |
| hf | -1061.51 | kJ/mol | Joback Method |
| hfus | 60.64 | kJ/mol | Joback Method |
| hvap | 93.74 | kJ/mol | Joback Method |
| log10ws | -8.37 | | Crippen Method |
| logp | 7.769 | | Crippen Method |
| mcvol | 395.310 | ml/mol | McGowan Method |
| pc | 798.89 | kPa | Joback Method |
| rinpol | 2851.00 | | NIST Webbook |
| rinpol | 2851.00 | | NIST Webbook |
| tb | 984.18 | K | Joback Method |
| tc | 1206.59 | K | Joback Method |
| tf | 526.51 | K | Joback Method |
| vc | 1.522 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1410.73 | J/mol×K | 984.18 | Joback Method |
| cpg | 1492.66 | J/mol×K | 1169.52 | Joback Method |
| cpg | 1480.00 | J/mol×K | 1132.45 | Joback Method |
| cpg | 1465.52 | J/mol×K | 1095.39 | Joback Method |
| cpg | 1449.19 | J/mol×K | 1058.32 | Joback Method |
| cpg | 1430.94 | J/mol×K | 1021.25 | Joback Method |
| cpg | 1503.56 | J/mol×K | 1206.59 | Joback Method |
| dvisc | 0.0000231 | Pa×s | 984.18 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000312 | Pa×s | 907.90 | Joback Method |
| dvisc | 0.0000444 | Pa×s | 831.62 | Joback Method |
| dvisc | 0.0000680 | Pa×s | 755.35 | Joback Method |
| dvisc | 0.0001144 | Pa×s | 679.07 | Joback Method |
| dvisc | 0.0002198 | Pa×s | 602.79 | Joback Method |
| dvisc | 0.0005103 | Pa×s | 526.51 | Joback Method |

# Sources

| | |
|---|---|
| **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=U339526&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |