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

**Inchi:** InChI=1S/C29H48O4/c1-2-3-4-5-6-7-8-9-12-15-32-28(30)25-13-10-11-14-26(25)29(31)33

**InchiKey:** VYMVOHWZEPGDKT-UHFFFAOYSA-N

**Formula:** C29H48O4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3

**Mol. weight [g/mol]:** 460.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -103.07 | kJ/mol | Joback Method |
| hf | -925.95 | kJ/mol | Joback Method |
| hfus | 63.79 | kJ/mol | Joback Method |
| hvap | 97.87 | kJ/mol | Joback Method |
| log10ws | -7.93 | | Crippen Method |
| logp | 7.235 | | Crippen Method |
| mcvol | 390.910 | ml/mol | McGowan Method |
| pc | 870.68 | kPa | Joback Method |
| rinpol | 3407.00 | | NIST Webbook |
| rinpol | 3407.00 | | NIST Webbook |
| tb | 1045.53 | K | Joback Method |
| tc | 1280.07 | K | Joback Method |
| tf | 605.87 | K | Joback Method |
| vc | 1.500 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1503.20 | J/mol×K | 1045.53 | Joback Method |
| cpg | 1524.18 | J/mol×K | 1084.62 | Joback Method |
| cpg | 1543.56 | J/mol×K | 1123.71 | Joback Method |
| cpg | 1561.48 | J/mol×K | 1162.80 | Joback Method |
| cpg | 1578.09 | J/mol×K | 1201.89 | Joback Method |
| cpg | 1593.52 | J/mol×K | 1240.98 | Joback Method |
| cpg | 1607.92 | J/mol×K | 1280.07 | Joback Method |
| dvisc | 0.0034701 | Pa×s | 605.87 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0025074 | Pa×s | 679.15 | Joback Method |
| dvisc | 0.0019301 | Pa×s | 752.42 | Joback Method |
| dvisc | 0.0015564 | Pa×s | 825.70 | Joback Method |
| dvisc | 0.0012998 | Pa×s | 898.98 | Joback Method |
| dvisc | 0.0011155 | Pa×s | 972.25 | Joback Method |
| dvisc | 0.0009780 | Pa×s | 1045.53 | 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=U339776&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 |