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

**Inchi:** InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-16-21-31-27(29)24-18-12-13-19-25(24)28(30)
**InchiKey:** VUHYXHMIUVGZJF-UHFFFAOYSA-N
**Formula:** C28H44O4
**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C
**Mol. weight [g/mol]:** 444.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -165.88 | kJ/mol | Joback Method |
| hf | -857.09 | kJ/mol | Joback Method |
| hfus | 56.88 | kJ/mol | Joback Method |
| hvap | 98.90 | kJ/mol | Joback Method |
| log10ws | -8.36 | | Crippen Method |
| logp | 7.596 | | Crippen Method |
| mcvol | 385.640 | ml/mol | McGowan Method |
| pc | 908.34 | kPa | Joback Method |
| rinpol | 3115.00 | | NIST Webbook |
| rinpol | 3115.00 | | NIST Webbook |
| tb | 1038.72 | K | Joback Method |
| tc | 1271.69 | K | Joback Method |
| tf | 576.72 | K | Joback Method |
| vc | 1.470 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1368.17 | J/mol×K | 1038.72 | Joback Method |
| cpg | 1384.71 | J/mol×K | 1077.55 | Joback Method |
| cpg | 1399.24 | J/mol×K | 1116.38 | Joback Method |
| cpg | 1411.83 | J/mol×K | 1155.20 | Joback Method |
| cpg | 1422.54 | J/mol×K | 1194.03 | Joback Method |
| cpg | 1431.44 | J/mol×K | 1232.86 | Joback Method |
| cpg | 1438.57 | J/mol×K | 1271.69 | Joback Method |
| dvisc | 0.0003344 | Pa×s | 576.72 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001610 | Pa×s | 653.72 | Joback Method |
| dvisc | 0.0000904 | Pa×s | 730.72 | Joback Method |
| dvisc | 0.0000567 | Pa×s | 807.72 | Joback Method |
| dvisc | 0.0000385 | Pa×s | 884.72 | Joback Method |
| dvisc | 0.0000279 | Pa×s | 961.72 | Joback Method |
| dvisc | 0.0000211 | Pa×s | 1038.72 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U339705&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 |

# 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 |