# 1,2-Cyclohexanedicarboxylic acid, 3-methylbut-2-yl undecyl ester

**Inchi:** InChI=1S/C24H44O4/c1-5-6-7-8-9-10-11-12-15-18-27-23(25)21-16-13-14-17-22(21)24(2

**InchiKey:** YFNMYKRTSXUWEE-UHFFFAOYSA-N

**Formula:** C24H44O4

**SMILES:** CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

**Mol. weight [g/mol]:** 396.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -304.78 | kJ/mol | Joback Method |
| hf | -1004.87 | kJ/mol | Joback Method |
| hfus | 49.35 | kJ/mol | Joback Method |
| hvap | 86.67 | kJ/mol | Joback Method |
| log10ws | -6.88 | | Crippen Method |
| logp | 6.454 | | Crippen Method |
| mcvol | 353.040 | ml/mol | McGowan Method |
| pc | 951.42 | kPa | Joback Method |
| rinpol | 2645.00 | | NIST Webbook |
| tb | 915.10 | K | Joback Method |
| tc | 1121.60 | K | Joback Method |
| tf | 477.70 | K | Joback Method |
| vc | 1.347 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1219.56 | J/mol×K | 915.10 | Joback Method |
| cpg | 1239.32 | J/mol×K | 949.52 | Joback Method |
| cpg | 1257.45 | J/mol×K | 983.93 | Joback Method |
| cpg | 1273.97 | J/mol×K | 1018.35 | Joback Method |
| cpg | 1288.91 | J/mol×K | 1052.77 | Joback Method |
| cpg | 1302.30 | J/mol×K | 1087.18 | Joback Method |
| cpg | 1314.18 | J/mol×K | 1121.60 | Joback Method |
| dvisc | 0.0008669 | Pa×s | 477.70 | Joback Method |
| dvisc | 0.0003513 | Pa×s | 550.60 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001758 | Pa×s | 623.50 | Joback Method |
| dvisc | 0.0001017 | Pa×s | 696.40 | Joback Method |
| dvisc | 0.0000653 | Pa×s | 769.30 | Joback Method |
| dvisc | 0.0000452 | Pa×s | 842.20 | Joback Method |
| dvisc | 0.0000332 | Pa×s | 915.10 | Joback Method |

# Sources

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|---|---|
| **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=U339564&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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