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

**Inchi:** InChI=1S/C31H58O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-30(32)28-2

**InchiKey:** GSTYJNGWJWKTLP-UHFFFAOYSA-N

**Formula:** C31H58O4

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

**Mol. weight [g/mol]:** 494.79

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -245.84 | kJ/mol | Joback Method |
| hf | -1149.35 | kJ/mol | Joback Method |
| hfus | 67.48 | kJ/mol | Joback Method |
| hvap | 102.26 | kJ/mol | Joback Method |
| log10ws | -9.81 | | Crippen Method |
| logp | 9.185 | | Crippen Method |
| mcvol | 451.670 | ml/mol | McGowan Method |
| pc | 652.77 | kPa | Joback Method |
| rinpol | 3385.00 | | NIST Webbook |
| rinpol | 3385.00 | | NIST Webbook |
| tb | 1075.26 | K | Joback Method |
| tc | 1333.40 | K | Joback Method |
| tf | 556.59 | K | Joback Method |
| vc | 1.740 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1669.80 | J/mol×K | 1075.26 | Joback Method |
| cpg | 1690.68 | J/mol×K | 1118.28 | Joback Method |
| cpg | 1708.85 | J/mol×K | 1161.31 | Joback Method |
| cpg | 1724.42 | J/mol×K | 1204.33 | Joback Method |
| cpg | 1737.50 | J/mol×K | 1247.36 | Joback Method |
| cpg | 1748.18 | J/mol×K | 1290.38 | Joback Method |
| cpg | 1756.56 | J/mol×K | 1333.40 | Joback Method |
| dvisc | 0.0003337 | Pa×s | 556.59 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001295 | Pa×s | 643.04 | Joback Method |
| dvisc | 0.0000629 | Pa×s | 729.48 | Joback Method |
| dvisc | 0.0000356 | Pa×s | 815.92 | Joback Method |
| dvisc | 0.0000225 | Pa×s | 902.37 | Joback Method |
| dvisc | 0.0000154 | Pa×s | 988.82 | Joback Method |
| dvisc | 0.0000112 | Pa×s | 1075.26 | 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=U339570&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 |