# cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl pentadecyl ester

**Inchi:** InChI=1S/C29H52O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-21-25-33-29(31)27-23-19-18-

**InchiKey:** KSMJSJUOMLUMGF-UHFFFAOYSA-N

**Formula:** C29H52O4

**SMILES:** CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCC

**Mol. weight [g/mol]:** 464.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -227.84 | kJ/mol | Joback Method |
| hf | -1039.73 | kJ/mol | Joback Method |
| hfus | 70.57 | kJ/mol | Joback Method |
| hvap | 98.87 | kJ/mol | Joback Method |
| log10ws | -8.95 | | Crippen Method |
| logp | 8.327 | | Crippen Method |
| mcvol | 419.190 | ml/mol | McGowan Method |
| pc | 729.67 | kPa | Joback Method |
| rinpol | 3189.00 | | NIST Webbook |
| rinpol | 3189.00 | | NIST Webbook |
| tb | 1029.54 | K | Joback Method |
| tc | 1269.23 | K | Joback Method |
| tf | 564.81 | K | Joback Method |
| vc | 1.625 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1507.35 | J/mol×K | 1029.54 | Joback Method |
| cpg | 1527.56 | J/mol×K | 1069.49 | Joback Method |
| cpg | 1545.56 | J/mol×K | 1109.44 | Joback Method |
| cpg | 1561.43 | J/mol×K | 1149.39 | Joback Method |
| cpg | 1575.24 | J/mol×K | 1189.34 | Joback Method |
| cpg | 1587.06 | J/mol×K | 1229.28 | Joback Method |
| cpg | 1596.97 | J/mol×K | 1269.23 | Joback Method |
| dvisc | 0.0003529 | Pa×s | 564.81 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001651 | Pa×s | 642.26 | Joback Method |
| dvisc | 0.0000909 | Pa×s | 719.72 | Joback Method |
| dvisc | 0.0000563 | Pa×s | 797.17 | Joback Method |
| dvisc | 0.0000379 | Pa×s | 874.63 | Joback Method |
| dvisc | 0.0000272 | Pa×s | 952.08 | Joback Method |
| dvisc | 0.0000205 | Pa×s | 1029.54 | Joback Method |

# Sources

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|---|---|
| **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=U382671&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 |