

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

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| Inchi: | InChI=1S/C28H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-20-24-32-28(30)26-22-18-17-21- |
| InchiKey: | LTJRTGSDUMFNDS-UHFFFAOYSA-N |
| Formula: | C28H50O4 |
| SMILES: | CCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC |
| Mol. weight [g/mol]: | 450.69 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -236.26 | kJ/mol | Joback Method |
| hf | -1019.09 | kJ/mol | Joback Method |
| hfus | 67.98 | kJ/mol | Joback Method |
| hvap | 96.65 | kJ/mol | Joback Method |
| log10ws | -8.53 | | Crippen Method |
| logp | 7.937 | | Crippen Method |
| mcvol | 405.100 | ml/mol | McGowan Method |
| pc | 769.04 | kPa | Joback Method |
| rinpol | 3088.00 | | NIST Webbook |
| rinpol | 3088.00 | | NIST Webbook |
| tb | 1006.66 | K | Joback Method |
| tc | 1237.24 | K | Joback Method |
| tf | 553.54 | K | Joback Method |
| vc | 1.569 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1443.01 | J/molxK | 1006.66 | Joback Method |
| cpg | 1462.94 | J/molxK | 1045.09 | Joback Method |
| cpg | 1480.83 | J/molxK | 1083.52 | Joback Method |
| cpg | 1496.76 | J/molxK | 1121.95 | Joback Method |
| cpg | 1510.76 | J/molxK | 1160.38 | Joback Method |
| cpg | 1522.92 | J/molxK | 1198.81 | Joback Method |
| cpg | 1533.29 | J/molxK | 1237.24 | Joback Method |
| dvisc | 0.0004005 | Paxs | 553.54 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0001889 | Paxs | 629.06 | Joback Method |
| dvisc | 0.0001047 | Paxs | 704.58 | Joback Method |
| dvisc | 0.0000651 | Paxs | 780.10 | Joback Method |
| dvisc | 0.0000440 | Paxs | 855.62 | Joback Method |
| dvisc | 0.0000317 | Paxs | 931.14 | Joback Method |
| dvisc | 0.0000239 | Paxs | 1006.66 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U382670&Units=SI |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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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<https://www.chemeo.com/cid/80-656-5/cis-Cyclohex-4-en-1-2-dicarboxylic-acid-hexyl-tetradecyl-ester.pdf>

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