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

**Inchi:** InChI=1S/C23H40O4/c1-3-5-7-9-10-11-15-19-27-23(25)21-17-13-12-16-20(21)22(24)26-

**InchiKey:** LDXUUPHMXNQKPS-UHFFFAOYSA-N

**Formula:** C23H40O4

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

**Mol. weight [g/mol]:** 380.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -278.36 | kJ/mol | Joback Method |
| hf | -915.89 | kJ/mol | Joback Method |
| hfus | 55.03 | kJ/mol | Joback Method |
| hvap | 85.52 | kJ/mol | Joback Method |
| log10ws | -6.44 | | Crippen Method |
| logp | 5.986 | | Crippen Method |
| mcvol | 334.650 | ml/mol | McGowan Method |
| pc | 1023.34 | kPa | Joback Method |
| rinpol | 2579.00 | | NIST Webbook |
| tb | 892.26 | K | Joback Method |
| tc | 1094.33 | K | Joback Method |
| tf | 497.19 | K | Joback Method |
| vc | 1.290 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1126.05 | J/mol×K | 892.26 | Joback Method |
| cpg | 1144.95 | J/mol×K | 925.94 | Joback Method |
| cpg | 1162.38 | J/mol×K | 959.62 | Joback Method |
| cpg | 1178.38 | J/mol×K | 993.30 | Joback Method |
| cpg | 1192.96 | J/mol×K | 1026.97 | Joback Method |
| cpg | 1206.16 | J/mol×K | 1060.65 | Joback Method |
| cpg | 1218.01 | J/mol×K | 1094.33 | Joback Method |
| dvisc | 0.0007213 | Pa×s | 497.19 | Joback Method |
| dvisc | 0.0003567 | Pa×s | 563.03 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002044 | Pa×s | 628.88 | Joback Method |
| dvisc | 0.0001302 | Pa×s | 694.73 | Joback Method |
| dvisc | 0.0000897 | Pa×s | 760.57 | Joback Method |
| dvisc | 0.0000655 | Pa×s | 826.42 | Joback Method |
| dvisc | 0.0000502 | Pa×s | 892.26 | Joback Method |

# Sources

**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=U382666&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