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

**Inchi:** InChI=1S/C20H34O4/c1-4-5-6-9-14-23-19(21)17-12-7-8-13-18(17)20(22)24-15-10-11-16

**InchiKey:** XFGCMWFHQFHTJN-UHFFFAOYSA-N

**Formula:** C20H34O4

**SMILES:** CCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

**Mol. weight [g/mol]:** 338.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -306.06 | kJ/mol | Joback Method |
| hf | -859.25 | kJ/mol | Joback Method |
| hfus | 43.73 | kJ/mol | Joback Method |
| hvap | 78.45 | kJ/mol | Joback Method |
| log10ws | -4.94 | | Crippen Method |
| logp | 4.672 | | Crippen Method |
| mcvol | 292.380 | ml/mol | McGowan Method |
| pc | 1248.61 | kPa | Joback Method |
| rinpol | 2249.00 | | NIST Webbook |
| tb | 823.18 | K | Joback Method |
| tc | 1020.86 | K | Joback Method |
| tf | 448.38 | K | Joback Method |
| vc | 1.115 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 942.11 | J/mol×K | 823.18 | Joback Method |
| cpg | 1022.51 | J/mol×K | 987.91 | Joback Method |
| cpg | 1008.98 | J/mol×K | 954.96 | Joback Method |
| cpg | 994.20 | J/mol×K | 922.02 | Joback Method |
| cpg | 978.14 | J/mol×K | 889.07 | Joback Method |
| cpg | 960.78 | J/mol×K | 856.13 | Joback Method |
| cpg | 1034.79 | J/mol×K | 1020.86 | Joback Method |
| dvisc | 0.0000698 | Pa×s | 823.18 | Joback Method |
| dvisc | 0.0000918 | Pa×s | 760.71 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001268 | Pa×s | 698.25 | Joback Method |
| dvisc | 0.0001867 | Pa×s | 635.78 | Joback Method |
| dvisc | 0.0002991 | Pa×s | 573.31 | Joback Method |
| dvisc | 0.0005375 | Pa×s | 510.85 | Joback Method |
| dvisc | 0.0011375 | Pa×s | 448.38 | 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=U382663&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 |