# 1,2-Cyclohexanedicarboxylic acid, 2-ethoxyethyl octyl ester

**Inchi:** InChI=1S/C20H36O5/c1-3-5-6-7-8-11-14-24-19(21)17-12-9-10-13-18(17)20(22)25-16-15

**InchiKey:** ZBOOSQLTKNKYFY-UHFFFAOYSA-N

**Formula:** C20H36O5

**SMILES:** CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC

**Mol. weight [g/mol]:** 356.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -438.58 | kJ/mol | Joback Method |
| hf | -1043.97 | kJ/mol | Joback Method |
| hfus | 47.22 | kJ/mol | Joback Method |
| hvap | 80.96 | kJ/mol | Joback Method |
| log10ws | -4.42 | | Crippen Method |
| logp | 4.276 | | Crippen Method |
| mcvol | 302.550 | ml/mol | McGowan Method |
| pc | 1196.48 | kPa | Joback Method |
| rinpol | 2390.00 | | NIST Webbook |
| rinpol | 2390.00 | | NIST Webbook |
| tb | 846.88 | K | Joback Method |
| tc | 1043.91 | K | Joback Method |
| tf | 484.85 | K | Joback Method |
| vc | 1.153 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1001.22 | J/mol×K | 846.88 | Joback Method |
| cpg | 1080.68 | J/mol×K | 1011.07 | Joback Method |
| cpg | 1067.58 | J/mol×K | 978.23 | Joback Method |
| cpg | 1053.09 | J/mol×K | 945.40 | Joback Method |
| cpg | 1037.20 | J/mol×K | 912.56 | Joback Method |
| cpg | 1019.91 | J/mol×K | 879.72 | Joback Method |
| cpg | 1092.41 | J/mol×K | 1043.91 | Joback Method |
| dvisc | 0.0000531 | Pa×s | 846.88 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000692 | Pa×s | 786.54 | Joback Method |
| dvisc | 0.0000943 | Pa×s | 726.20 | Joback Method |
| dvisc | 0.0001360 | Pa×s | 665.87 | Joback Method |
| dvisc | 0.0002108 | Pa×s | 605.53 | Joback Method |
| dvisc | 0.0003600 | Pa×s | 545.19 | Joback Method |
| dvisc | 0.0007025 | Pa×s | 484.85 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U339910&Units=SI |
| **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 |

# 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 |