# 1,2-Cyclohexanedicarboxylic acid, difurfuryl ester

**Inchi:** InChI=1S/C18H28O6/c19-17(23-11-13-5-3-9-21-13)15-7-1-2-8-16(15)18(20)24-12-14-6-4-10-22-14/h13-16H,1-12H2

**InchiKey:** YKLOZNRRBGPWAL-UHFFFAOYSA-N

**Formula:** C18H28O6

**SMILES:** O=C(OCC1CCCO1)C1CCCCC1C(=O)OCC1CCCO1

**Mol. weight [g/mol]:** 340.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -449.56 | kJ/mol | Joback Method |
| hf | -1013.51 | kJ/mol | Joback Method |
| hfus | 44.68 | kJ/mol | Joback Method |
| hvap | 83.63 | kJ/mol | Joback Method |
| log10ws | -2.68 | | Crippen Method |
| logp | 2.237 | | Crippen Method |
| mcvol | 258.520 | ml/mol | McGowan Method |
| pc | 1826.28 | kPa | Joback Method |
| rinpol | 2576.00 | | NIST Webbook |
| rinpol | 2576.00 | | NIST Webbook |
| tb | 863.16 | K | Joback Method |
| tc | 1093.97 | K | Joback Method |
| tf | 515.02 | K | Joback Method |
| vc | 0.948 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 902.13 | J/mol×K | 863.16 | Joback Method |
| cpg | 920.86 | J/mol×K | 901.63 | Joback Method |
| cpg | 937.72 | J/mol×K | 940.10 | Joback Method |
| cpg | 952.76 | J/mol×K | 978.56 | Joback Method |
| cpg | 966.03 | J/mol×K | 1017.03 | Joback Method |
| cpg | 977.55 | J/mol×K | 1055.50 | Joback Method |
| cpg | 987.38 | J/mol×K | 1093.97 | Joback Method |
| dvisc | 0.0014965 | Pa×s | 515.02 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0008472 | Pa×s | 573.04 | Joback Method |
| dvisc | 0.0005325 | Pa×s | 631.07 | Joback Method |
| dvisc | 0.0003619 | Pa×s | 689.09 | Joback Method |
| dvisc | 0.0002612 | Pa×s | 747.11 | Joback Method |
| dvisc | 0.0001976 | Pa×s | 805.14 | Joback Method |
| dvisc | 0.0001552 | Pa×s | 863.16 | Joback Method |

# Sources

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|---|---|
| **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=U339906&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |