# 1,2-Cyclohexanedicarboxylic acid, ethyl 4-methoxyphenyl ester

**Inchi:** InChI=1S/C17H22O5/c1-3-21-16(18)14-6-4-5-7-15(14)17(19)22-13-10-8-12(20-2)9-11-13

**InchiKey:** LAGULUFALMQLGT-UHFFFAOYSA-N

**Formula:** C17H22O5

**SMILES:** CCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC)cc1

**Mol. weight [g/mol]:** 306.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -361.06 | kJ/mol | Joback Method |
| hf | -756.99 | kJ/mol | Joback Method |
| hfus | 33.11 | kJ/mol | Joback Method |
| hvap | 77.22 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 2.970 | | Crippen Method |
| mcvol | 236.520 | ml/mol | McGowan Method |
| pc | 1911.91 | kPa | Joback Method |
| rinpol | 2323.00 | | NIST Webbook |
| tb | 809.90 | K | Joback Method |
| tc | 1034.03 | K | Joback Method |
| tf | 489.98 | K | Joback Method |
| vc | 0.877 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 730.60 | J/mol×K | 809.90 | Joback Method |
| cpg | 747.36 | J/mol×K | 847.26 | Joback Method |
| cpg | 762.61 | J/mol×K | 884.61 | Joback Method |
| cpg | 776.33 | J/mol×K | 921.97 | Joback Method |
| cpg | 788.53 | J/mol×K | 959.32 | Joback Method |
| cpg | 799.21 | J/mol×K | 996.68 | Joback Method |
| cpg | 808.35 | J/mol×K | 1034.03 | Joback Method |
| dvisc | 0.0006881 | Pa×s | 489.98 | Joback Method |
| dvisc | 0.0004064 | Pa×s | 543.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002637 | Pa×s | 596.62 | Joback Method |
| dvisc | 0.0001837 | Pa×s | 649.94 | Joback Method |
| dvisc | 0.0001352 | Pa×s | 703.26 | Joback Method |
| dvisc | 0.0001039 | Pa×s | 756.58 | Joback Method |
| dvisc | 0.0000827 | Pa×s | 809.90 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U339666&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 |