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

**Inchi:** InChI=1S/C22H32O5/c1-3-4-5-6-9-16-26-21(23)19-10-7-8-11-20(19)22(24)27-18-14-12-1

**InchiKey:** BIROOVPAKYONCK-UHFFFAOYSA-N

**Formula:** C22H32O5

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

**Mol. weight [g/mol]:** 376.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -318.96 | kJ/mol | Joback Method |
| hf | -860.19 | kJ/mol | Joback Method |
| hfus | 46.06 | kJ/mol | Joback Method |
| hvap | 88.35 | kJ/mol | Joback Method |
| log10ws | -5.62 | | Crippen Method |
| logp | 4.921 | | Crippen Method |
| mcvol | 306.970 | ml/mol | McGowan Method |
| pc | 1306.12 | kPa | Joback Method |
| rinpol | 2794.00 | | NIST Webbook |
| rinpol | 2794.00 | | NIST Webbook |
| tb | 924.30 | K | Joback Method |
| tc | 1142.61 | K | Joback Method |
| tf | 546.33 | K | Joback Method |
| vc | 1.157 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1026.24 | J/mol×K | 924.30 | Joback Method |
| cpg | 1090.27 | J/mol×K | 1106.22 | Joback Method |
| cpg | 1080.84 | J/mol×K | 1069.84 | Joback Method |
| cpg | 1069.73 | J/mol×K | 1033.45 | Joback Method |
| cpg | 1056.94 | J/mol×K | 997.07 | Joback Method |
| cpg | 1042.45 | J/mol×K | 960.68 | Joback Method |
| cpg | 1098.04 | J/mol×K | 1142.61 | Joback Method |
| dvisc | 0.0000418 | Pa×s | 924.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000535 | Pa×s | 861.30 | Joback Method |
| dvisc | 0.0000710 | Pa×s | 798.31 | Joback Method |
| dvisc | 0.0000990 | Pa×s | 735.31 | Joback Method |
| dvisc | 0.0001470 | Pa×s | 672.32 | Joback Method |
| dvisc | 0.0002367 | Pa×s | 609.32 | Joback Method |
| dvisc | 0.0004256 | Pa×s | 546.33 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U339672&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 |

# 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 |