# 1,2-Cyclohexanedicarboxylic acid, heptyl 3-phenylpropyl ester

**Inchi:** InChI=1S/C24H36O4/c1-2-3-4-5-11-18-27-23(25)21-16-9-10-17-22(21)24(26)28-19-12-1

**InchiKey:** NILXROAMBOTYBR-UHFFFAOYSA-N

**Formula:** C24H36O4

**SMILES:** CCCCCCCOC(=O)C1CCCCC1C(=O)OCCCc1ccccc1

**Mol. weight [g/mol]:** 388.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -187.49 | kJ/mol | Joback Method |
| hf | -757.78 | kJ/mol | Joback Method |
| hfus | 50.44 | kJ/mol | Joback Method |
| hvap | 89.73 | kJ/mol | Joback Method |
| log10ws | -6.11 | | Crippen Method |
| logp | 5.482 | | Crippen Method |
| mcvol | 329.280 | ml/mol | McGowan Method |
| pc | 1167.22 | kPa | Joback Method |
| rinpol | 2839.00 | | NIST Webbook |
| rinpol | 2839.00 | | NIST Webbook |
| tb | 942.66 | K | Joback Method |
| tc | 1160.85 | K | Joback Method |
| tf | 534.12 | K | Joback Method |
| vc | 1.252 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1119.58 | J/mol×K | 942.66 | Joback Method |
| cpg | 1136.66 | J/mol×K | 979.02 | Joback Method |
| cpg | 1152.09 | J/mol×K | 1015.39 | Joback Method |
| cpg | 1165.89 | J/mol×K | 1051.75 | Joback Method |
| cpg | 1178.12 | J/mol×K | 1088.12 | Joback Method |
| cpg | 1188.83 | J/mol×K | 1124.48 | Joback Method |
| cpg | 1198.05 | J/mol×K | 1160.85 | Joback Method |
| dvisc | 0.0005604 | Pa×s | 534.12 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002836 | Pa×s | 602.21 | Joback Method |
| dvisc | 0.0001648 | Pa×s | 670.30 | Joback Method |
| dvisc | 0.0001059 | Pa×s | 738.39 | Joback Method |
| dvisc | 0.0000733 | Pa×s | 806.48 | Joback Method |
| dvisc | 0.0000537 | Pa×s | 874.57 | Joback Method |
| dvisc | 0.0000412 | Pa×s | 942.66 | Joback Method |

# Sources

| | |
|---|---|
| **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=U339498&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 |