# cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl heptyl ester

**Inchi:** InChI=1S/C22H29ClO4/c1-3-4-5-6-9-14-26-21(24)18-10-7-8-11-19(18)22(25)27-17-12-13

**InchiKey:** KDFROPAKHRGPHZ-UHFFFAOYSA-N

**Formula:** C22H29ClO4

**SMILES:** CCCCCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1

**Mol. weight [g/mol]:** 392.92

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -205.56 | kJ/mol | Joback Method |
| hf | -697.40 | kJ/mol | Joback Method |
| hfus | 49.90 | kJ/mol | Joback Method |
| hvap | 91.27 | kJ/mol | Joback Method |
| log10ws | -6.52 | | Crippen Method |
| logp | 5.650 | | Crippen Method |
| mcvol | 309.040 | ml/mol | McGowan Method |
| pc | 1307.06 | kPa | Joback Method |
| rinpol | 2808.00 | | NIST Webbook |
| rinpol | 2808.00 | | NIST Webbook |
| tb | 943.45 | K | Joback Method |
| tc | 1167.27 | K | Joback Method |
| tf | 567.30 | K | Joback Method |
| vc | 1.175 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 991.76 | J/mol×K | 943.45 | Joback Method |
| cpg | 1006.49 | J/mol×K | 980.75 | Joback Method |
| cpg | 1019.63 | J/mol×K | 1018.06 | Joback Method |
| cpg | 1031.22 | J/mol×K | 1055.36 | Joback Method |
| cpg | 1041.28 | J/mol×K | 1092.67 | Joback Method |
| cpg | 1049.84 | J/mol×K | 1129.97 | Joback Method |
| cpg | 1056.93 | J/mol×K | 1167.27 | Joback Method |
| dvisc | 0.0004423 | Pa×s | 567.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002613 | Pa×s | 629.99 | Joback Method |
| dvisc | 0.0001698 | Pa×s | 692.68 | Joback Method |
| dvisc | 0.0001185 | Pa×s | 755.38 | Joback Method |
| dvisc | 0.0000874 | Pa×s | 818.07 | Joback Method |
| dvisc | 0.0000673 | Pa×s | 880.76 | Joback Method |
| dvisc | 0.0000537 | Pa×s | 943.45 | 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=U382652&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