# Carbonic acid, neopentyl 4-chlorophenyl ester

**Inchi:** InChI=1S/C12H15ClO3/c1-12(2,3)8-15-11(14)16-10-6-4-9(13)5-7-10/h4-7H,8H2,1-3H3
**InchiKey:** NYJHHOFKZJVGJQ-UHFFFAOYSA-N
**Formula:** C12H15ClO3
**SMILES:** CC(C)(C)COC(=O)Oc1ccc(Cl)cc1
**Mol. weight [g/mol]:** 242.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -195.07 | kJ/mol | Joback Method |
| hf | -467.46 | kJ/mol | Joback Method |
| hfus | 21.25 | kJ/mol | Joback Method |
| hvap | 59.90 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.901 | | Crippen Method |
| mcvol | 181.730 | ml/mol | McGowan Method |
| pc | 2395.87 | kPa | Joback Method |
| rinpol | 1593.00 | | NIST Webbook |
| rinpol | 1593.00 | | NIST Webbook |
| tb | 638.53 | K | Joback Method |
| tc | 859.03 | K | Joback Method |
| tf | 390.67 | K | Joback Method |
| vc | 0.679 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 449.77 | J/mol×K | 638.53 | Joback Method |
| cpg | 464.12 | J/mol×K | 675.28 | Joback Method |
| cpg | 477.51 | J/mol×K | 712.03 | Joback Method |
| cpg | 489.98 | J/mol×K | 748.78 | Joback Method |
| cpg | 501.55 | J/mol×K | 785.53 | Joback Method |
| cpg | 512.25 | J/mol×K | 822.28 | Joback Method |
| cpg | 522.10 | J/mol×K | 859.03 | Joback Method |
| dvisc | 0.0011963 | Pa×s | 390.67 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006772 | Pa×s | 431.98 | Joback Method |
| dvisc | 0.0004234 | Pa×s | 473.29 | Joback Method |
| dvisc | 0.0002854 | Pa×s | 514.60 | Joback Method |
| dvisc | 0.0002040 | Pa×s | 555.91 | Joback Method |
| dvisc | 0.0001528 | Pa×s | 597.22 | Joback Method |
| dvisc | 0.0001188 | Pa×s | 638.53 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357860&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

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|---|---|
| **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 |