# 4-Chlorobutyric acid, 2,3-dimethylphenyl ester

**Inchi:** InChI=1S/C12H15ClO2/c1-9-5-3-6-11(10(9)2)15-12(14)7-4-8-13/h3,5-6H,4,7-8H2,1-2H3
**InchiKey:** JDPZPTASAVCWGW-UHFFFAOYSA-N
**Formula:** C12H15ClO2
**SMILES:** Cc1cccc(OC(=O)CCCCl)c1C
**Mol. weight [g/mol]:** 226.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -102.54 | kJ/mol | Joback Method |
| hf | -337.96 | kJ/mol | Joback Method |
| hfus | 27.08 | kJ/mol | Joback Method |
| hvap | 59.45 | kJ/mol | Joback Method |
| log10ws | -3.73 | | Crippen Method |
| logp | 3.228 | | Crippen Method |
| mcvol | 175.860 | ml/mol | McGowan Method |
| pc | 2356.49 | kPa | Joback Method |
| rinpol | 1749.00 | | NIST Webbook |
| rinpol | 1749.00 | | NIST Webbook |
| tb | 624.32 | K | Joback Method |
| tc | 836.12 | K | Joback Method |
| tf | 378.54 | K | Joback Method |
| vc | 0.672 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 420.60 | J/mol×K | 624.32 | Joback Method |
| cpg | 481.99 | J/mol×K | 800.82 | Joback Method |
| cpg | 471.22 | J/mol×K | 765.52 | Joback Method |
| cpg | 459.71 | J/mol×K | 730.22 | Joback Method |
| cpg | 447.44 | J/mol×K | 694.92 | Joback Method |
| cpg | 434.41 | J/mol×K | 659.62 | Joback Method |
| cpg | 492.04 | J/mol×K | 836.12 | Joback Method |
| dvisc | 0.0001712 | Pa×s | 624.32 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002123 | Pa×s | 583.36 | Joback Method |
| dvisc | 0.0002718 | Pa×s | 542.39 | Joback Method |
| dvisc | 0.0003625 | Pa×s | 501.43 | Joback Method |
| dvisc | 0.0005088 | Pa×s | 460.47 | Joback Method |
| dvisc | 0.0007630 | Pa×s | 419.50 | Joback Method |
| dvisc | 0.0012490 | Pa×s | 378.54 | Joback Method |

# Sources

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|---|---|
| **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=U360643&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |