# 2-Chloropropionic acid, 3-methylphenyl ester

**Inchi:** InChI=1S/C10H11ClO2/c1-7-4-3-5-9(6-7)13-10(12)8(2)11/h3-6,8H,1-2H3
**InchiKey:** PAAIIYQEPLSEAS-UHFFFAOYSA-N
**Formula:** C10H11ClO2
**SMILES:** Cc1cccc(OC(=O)C(C)Cl)c1
**Mol. weight [g/mol]:** 198.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -112.19 | kJ/mol | Joback Method |
| hf | -290.49 | kJ/mol | Joback Method |
| hfus | 18.77 | kJ/mol | Joback Method |
| hvap | 53.95 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.528 | | Crippen Method |
| mcvol | 147.680 | ml/mol | McGowan Method |
| pc | 2937.70 | kPa | Joback Method |
| rinpol | 1426.00 | | NIST Webbook |
| rinpol | 1372.00 | | NIST Webbook |
| rinpol | 1426.00 | | NIST Webbook |
| tb | 573.14 | K | Joback Method |
| tc | 796.07 | K | Joback Method |
| tf | 328.48 | K | Joback Method |
| vc | 0.554 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 326.36 | J/mol×K | 573.14 | Joback Method |
| cpg | 339.19 | J/mol×K | 610.30 | Joback Method |
| cpg | 351.23 | J/mol×K | 647.45 | Joback Method |
| cpg | 362.51 | J/mol×K | 684.61 | Joback Method |
| cpg | 373.05 | J/mol×K | 721.76 | Joback Method |
| cpg | 382.87 | J/mol×K | 758.92 | Joback Method |
| cpg | 391.97 | J/mol×K | 796.07 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0020698 | Pa×s | 328.48 | Joback Method |
| dvisc | 0.0011257 | Pa×s | 369.26 | Joback Method |
| dvisc | 0.0006911 | Pa×s | 410.03 | Joback Method |
| dvisc | 0.0004634 | Pa×s | 450.81 | Joback Method |
| dvisc | 0.0003321 | Pa×s | 491.59 | Joback Method |
| dvisc | 0.0002504 | Pa×s | 532.36 | Joback Method |
| dvisc | 0.0001966 | Pa×s | 573.14 | 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=U307751&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 |