# 3-Chlorobenzoic acid, 4-chloro-2-methylphenyl ester

**Inchi:** InChI=1S/C14H10Cl2O2/c1-9-7-12(16)5-6-13(9)18-14(17)10-3-2-4-11(15)8-10/h2-8H,1H

**InchiKey:** BHLWDJNYZGNVBZ-UHFFFAOYSA-N

**Formula:** C14H10Cl2O2

**SMILES:** Cc1cc(Cl)ccc1OC(=O)c1cccc(Cl)c1

**Mol. weight [g/mol]:** 281.13

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 5.15 | kJ/mol | Joback Method |
| hf | -169.92 | kJ/mol | Joback Method |
| hfus | 30.11 | kJ/mol | Joback Method |
| hvap | 71.22 | kJ/mol | Joback Method |
| log10ws | -5.40 | | Crippen Method |
| logp | 4.521 | | Crippen Method |
| mcvol | 192.520 | ml/mol | McGowan Method |
| pc | 2568.89 | kPa | Joback Method |
| rinpol | 2155.00 | | NIST Webbook |
| tb | 739.17 | K | Joback Method |
| tc | 989.16 | K | Joback Method |
| tf | 469.94 | K | Joback Method |
| vc | 0.726 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 459.79 | J/mol×K | 739.17 | Joback Method |
| cpg | 472.01 | J/mol×K | 780.84 | Joback Method |
| cpg | 483.16 | J/mol×K | 822.50 | Joback Method |
| cpg | 493.27 | J/mol×K | 864.17 | Joback Method |
| cpg | 502.38 | J/mol×K | 905.83 | Joback Method |
| cpg | 510.53 | J/mol×K | 947.50 | Joback Method |
| cpg | 517.76 | J/mol×K | 989.16 | Joback Method |
| dvisc | 0.0007416 | Pa×s | 469.94 | Joback Method |
| dvisc | 0.0004884 | Pa×s | 514.81 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003439 | Pa×s | 559.68 | Joback Method |
| dvisc | 0.0002551 | Pa×s | 604.56 | Joback Method |
| dvisc | 0.0001972 | Pa×s | 649.43 | Joback Method |
| dvisc | 0.0001576 | Pa×s | 694.30 | Joback Method |
| dvisc | 0.0001294 | Pa×s | 739.17 | Joback Method |

# Sources

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|---|---|
| **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=U357399&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 |

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