# 3-Chlorobenzoic acid, isopropyl ester

**Other names:** Benzoic acid, 3-chloro, isopropyl ester
**Inchi:** InChI=1S/C10H11ClO2/c1-7(2)13-10(12)8-4-3-5-9(11)6-8/h3-7H,1-2H3
**InchiKey:** WDIWPDMGFDKALY-UHFFFAOYSA-N
**Formula:** C10H11ClO2
**SMILES:** CC(C)OC(=O)c1cccc(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 | -3.35 | | Crippen Method |
| logp | 2.905 | | Crippen Method |
| mcvol | 147.680 | ml/mol | McGowan Method |
| pc | 2937.70 | kPa | Joback Method |
| rinpol | 1348.00 | | NIST Webbook |
| rinpol | 1376.00 | | NIST Webbook |
| rinpol | 1341.00 | | NIST Webbook |
| rinpol | 1369.00 | | NIST Webbook |
| rinpol | 1356.00 | | NIST Webbook |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1354.00 | | NIST Webbook |
| ripol | 1852.00 | | NIST Webbook |
| ripol | 1833.00 | | NIST Webbook |
| ripol | 1869.00 | | NIST Webbook |
| ripol | 1883.00 | | NIST Webbook |
| ripol | 1878.00 | | NIST Webbook |
| ripol | 1852.00 | | NIST Webbook |
| ripol | 1863.00 | | 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 |
| 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

**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=U357778&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |