# 3-Chloro-2-fluorobenzoic acid, phenylester

**Inchi:** InChI=1S/C13H8ClFO2/c14-11-8-4-7-10(12(11)15)13(16)17-9-5-2-1-3-6-9/h1-8H
**InchiKey:** JNBLJOFPYZIRPK-UHFFFAOYSA-N
**Formula:** C13H8ClFO2
**SMILES:** O=C(Oc1ccccc1)c1cccc(Cl)c1F
**Mol. weight [g/mol]:** 250.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.52 | kJ/mol | Joback Method |
| hf | -318.18 | kJ/mol | Joback Method |
| hfus | 26.79 | kJ/mol | Joback Method |
| hvap | 63.13 | kJ/mol | Joback Method |
| log10ws | -4.58 | | Crippen Method |
| logp | 3.698 | | Crippen Method |
| mcvol | 167.960 | ml/mol | McGowan Method |
| pc | 2859.68 | kPa | Joback Method |
| rinpol | 1890.00 | | NIST Webbook |
| tb | 673.15 | K | Joback Method |
| tc | 913.93 | K | Joback Method |
| tf | 416.82 | K | Joback Method |
| vc | 0.638 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 396.42 | J/mol×K | 673.15 | Joback Method |
| cpg | 408.77 | J/mol×K | 713.28 | Joback Method |
| cpg | 420.11 | J/mol×K | 753.41 | Joback Method |
| cpg | 430.47 | J/mol×K | 793.54 | Joback Method |
| cpg | 439.89 | J/mol×K | 833.67 | Joback Method |
| cpg | 448.41 | J/mol×K | 873.80 | Joback Method |
| cpg | 456.07 | J/mol×K | 913.93 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357724&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |