# 3-Chloro-2-fluorobenzoic acid, hexyl ester

**Inchi:** InChI=1S/C13H16ClFO2/c1-2-3-4-5-9-17-13(16)10-7-6-8-11(14)12(10)15/h6-8H,2-5,9H2
**InchiKey:** YFRSPDVBDUHKAP-UHFFFAOYSA-N
**Formula:** C13H16ClFO2
**SMILES:** CCCCCCOC(=O)c1cccc(Cl)c1F
**Mol. weight [g/mol]:** 258.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -288.93 | kJ/mol | Joback Method |
| hf | -554.71 | kJ/mol | Joback Method |
| hfus | 32.75 | kJ/mol | Joback Method |
| hvap | 60.86 | kJ/mol | Joback Method |
| log10ws | -4.82 | | Crippen Method |
| logp | 4.216 | | Crippen Method |
| mcvol | 191.720 | ml/mol | McGowan Method |
| pc | 2064.24 | kPa | Joback Method |
| rinpol | 1817.00 | | NIST Webbook |
| rinpol | 1817.00 | | NIST Webbook |
| tb | 646.47 | K | Joback Method |
| tc | 846.27 | K | Joback Method |
| tf | 390.40 | K | Joback Method |
| vc | 0.747 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 478.71 | J/mol×K | 646.47 | Joback Method |
| cpg | 492.49 | J/mol×K | 679.77 | Joback Method |
| cpg | 505.51 | J/mol×K | 713.07 | Joback Method |
| cpg | 517.78 | J/mol×K | 746.37 | Joback Method |
| cpg | 529.32 | J/mol×K | 779.67 | Joback Method |
| cpg | 540.13 | J/mol×K | 812.97 | Joback Method |
| cpg | 550.25 | J/mol×K | 846.27 | 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=U338883&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |