# 3-Chloro-2-fluorobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

**Inchi:** InChI=1S/C13H4Cl5FO2/c14-6-3-1-2-5(11(6)19)13(20)21-12-8(16)4-7(15)9(17)10(12)18/

**InchiKey:** VWPZGMVLINDTQY-UHFFFAOYSA-N

**Formula:** C13H4Cl5FO2

**SMILES:** O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1cccc(Cl)c1F

**Mol. weight [g/mol]:** 388.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -262.76 | kJ/mol | Joback Method |
| hf | -427.02 | kJ/mol | Joback Method |
| hfus | 42.03 | kJ/mol | Joback Method |
| hvap | 83.32 | kJ/mol | Joback Method |
| log10ws | -7.32 | | Crippen Method |
| logp | 6.312 | | Crippen Method |
| mcvol | 216.920 | ml/mol | McGowan Method |
| pc | 2315.84 | kPa | Joback Method |
| rinpol | 2541.00 | | NIST Webbook |
| rinpol | 2541.00 | | NIST Webbook |
| tb | 842.79 | K | Joback Method |
| tc | 1094.87 | K | Joback Method |
| tf | 586.58 | K | Joback Method |
| vc | 0.835 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 467.45 | J/mol×K | 842.79 | Joback Method |
| cpg | 474.84 | J/mol×K | 884.80 | Joback Method |
| cpg | 481.35 | J/mol×K | 926.82 | Joback Method |
| cpg | 487.01 | J/mol×K | 968.83 | Joback Method |
| cpg | 491.82 | J/mol×K | 1010.85 | Joback Method |
| cpg | 495.80 | J/mol×K | 1052.86 | Joback Method |
| cpg | 498.96 | J/mol×K | 1094.87 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360589&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **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 |