# 2-Fluorobenzoic acid, 3,4-dichlorophenyl ester

**Inchi:** InChI=1S/C13H7Cl2FO2/c14-10-6-5-8(7-11(10)15)18-13(17)9-3-1-2-4-12(9)16/h1-7H
**InchiKey:** ODWCIDDVKYMMDX-UHFFFAOYSA-N
**Formula:** C13H7Cl2FO2
**SMILES:** O=C(Oc1ccc(Cl)c(Cl)c1)c1ccccc1F
**Mol. weight [g/mol]:** 285.10

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -198.08 | kJ/mol | Joback Method |
| hf | -345.39 | kJ/mol | Joback Method |
| hfus | 30.60 | kJ/mol | Joback Method |
| hvap | 68.18 | kJ/mol | Joback Method |
| log10ws | -5.26 | | Crippen Method |
| logp | 4.352 | | Crippen Method |
| mcvol | 180.200 | ml/mol | McGowan Method |
| pc | 2707.03 | kPa | Joback Method |
| rinpol | 2012.00 | | NIST Webbook |
| rinpol | 2012.00 | | NIST Webbook |
| tb | 715.56 | K | Joback Method |
| tc | 959.61 | K | Joback Method |
| tf | 459.26 | K | Joback Method |
| vc | 0.688 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 416.98 | J/mol×K | 715.56 | Joback Method |
| cpg | 428.00 | J/mol×K | 756.24 | Joback Method |
| cpg | 438.06 | J/mol×K | 796.91 | Joback Method |
| cpg | 447.19 | J/mol×K | 837.59 | Joback Method |
| cpg | 455.42 | J/mol×K | 878.26 | Joback Method |
| cpg | 462.77 | J/mol×K | 918.94 | Joback Method |
| cpg | 469.29 | J/mol×K | 959.61 | Joback Method |

# Sources

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|---|---|
| **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=U307690&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |