# 2,6-Difluoro-3-methylbenzoic acid, 4-chlorophenyl ester

**Inchi:** InChI=1S/C14H9ClF2O2/c1-8-2-7-11(16)12(13(8)17)14(18)19-10-5-3-9(15)4-6-10/h2-7H

**InchiKey:** MZKJPBVMPYPFGX-UHFFFAOYSA-N

**Formula:** C14H9ClF2O2

**SMILES:** Cc1ccc(F)c(C(=O)Oc2ccc(Cl)cc2)c1F

**Mol. weight [g/mol]:** 282.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -382.17 | kJ/mol | Joback Method |
| hf | -557.87 | kJ/mol | Joback Method |
| hfus | 31.69 | kJ/mol | Joback Method |
| hvap | 65.86 | kJ/mol | Joback Method |
| log10ws | -5.38 | | Crippen Method |
| logp | 4.146 | | Crippen Method |
| mcvol | 183.820 | ml/mol | McGowan Method |
| pc | 2400.57 | kPa | Joback Method |
| rinpol | 1968.00 | | NIST Webbook |
| rinpol | 1968.00 | | NIST Webbook |
| tb | 705.26 | K | Joback Method |
| tc | 932.46 | K | Joback Method |
| tf | 453.72 | K | Joback Method |
| vc | 0.713 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 451.72 | J/mol×K | 705.26 | Joback Method |
| cpg | 463.72 | J/mol×K | 743.13 | Joback Method |
| cpg | 474.81 | J/mol×K | 780.99 | Joback Method |
| cpg | 485.03 | J/mol×K | 818.86 | Joback Method |
| cpg | 494.38 | J/mol×K | 856.73 | Joback Method |
| cpg | 502.89 | J/mol×K | 894.60 | Joback Method |
| cpg | 510.58 | J/mol×K | 932.46 | 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=U357682&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 |