# 2,6-Difluorobenzoic acid, 4-cyanophenyl ester

**Inchi:** InChI=1S/C14H7F2NO2/c15-11-2-1-3-12(16)13(11)14(18)19-10-6-4-9(8-17)5-7-10/h1-7H
**InchiKey:** MTEGUFJKGHQFPI-UHFFFAOYSA-N
**Formula:** C14H7F2NO2
**SMILES:** N#Cc1ccc(OC(=O)c2c(F)cccc2F)cc1
**Mol. weight [g/mol]:** 259.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -227.43 | kJ/mol | Joback Method |
| hf | -365.78 | kJ/mol | Joback Method |
| hfus | 29.38 | kJ/mol | Joback Method |
| hvap | 71.30 | kJ/mol | Joback Method |
| log10ws | -4.57 | | Crippen Method |
| logp | 3.056 | | Crippen Method |
| mcvol | 172.960 | ml/mol | McGowan Method |
| pc | 2465.36 | kPa | Joback Method |
| rinpol | 1879.00 | | NIST Webbook |
| tb | 764.93 | K | Joback Method |
| tc | 999.55 | K | Joback Method |
| tf | 476.27 | K | Joback Method |
| vc | 0.690 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 445.59 | J/mol×K | 764.93 | Joback Method |
| cpg | 455.75 | J/mol×K | 804.03 | Joback Method |
| cpg | 465.01 | J/mol×K | 843.14 | Joback Method |
| cpg | 473.38 | J/mol×K | 882.24 | Joback Method |
| cpg | 480.91 | J/mol×K | 921.34 | Joback Method |
| cpg | 487.61 | J/mol×K | 960.44 | Joback Method |
| cpg | 493.51 | J/mol×K | 999.55 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307560&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |

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