

# 2,5-Difluorobenzoic acid, 4-cyanophenyl ester

**Inchi:** InChI=1S/C14H7F2NO2/c15-10-3-6-13(16)12(7-10)14(18)19-11-4-1-9(8-17)2-5-11/h1-7H  
**InchiKey:** QOOVFWRGEHPLOF-UHFFFAOYSA-N  
**Formula:** C14H7F2NO2  
**SMILES:** N#Cc1ccc(OC(=O)c2cc(F)ccc2F)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
mvol	172.960	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	2001.00		NIST Webbook
tb	764.93	K	Joback Method
tc	999.55	K	Joback Method
tf	476.27	K	Joback Method
vc	0.690	m <sup>3</sup> /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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357584&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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