

# 2-Fluorobenzoic acid, 4-cyanophenyl ester

<b>Inchi:</b>	InChI=1S/C14H8FNO2/c15-13-4-2-1-3-12(13)14(17)18-11-7-5-10(9-16)6-8-11/h1-8H
<b>InchiKey:</b>	UVPMWZRFROFENN-UHFFFAOYSA-N
<b>Formula:</b>	C14H8FNO2
<b>SMILES:</b>	N#Cc1ccc(OC(=O)c2ccccc2F)cc1
<b>Mol. weight [g/mol]:</b>	241.22

## Physical Properties

Property code	Value	Unit	Source
gf	-22.99	kJ/mol	Joback Method
hf	-158.20	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	2.917		Crippen Method
mvol	171.190	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	760.68	K	Joback Method
tc	1004.63	K	Joback Method
tf	463.16	K	Joback Method
vc	0.671	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.52	J/mol×K	760.68	Joback Method
cpg	450.33	J/mol×K	801.34	Joback Method
cpg	460.14	J/mol×K	842.00	Joback Method
cpg	469.00	J/mol×K	882.66	Joback Method
cpg	476.94	J/mol×K	923.31	Joback Method
cpg	484.00	J/mol×K	963.97	Joback Method
cpg	490.21	J/mol×K	1004.63	Joback Method

# Sources

<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=U307689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307689&amp;Units=SI</a>
<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>

# 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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