

# 3-Chloro-2-fluorobenzoic acid, 4-cyanophenyl ester

Inchi:	InChI=1S/C14H7ClFNO2/c15-12-3-1-2-11(13(12)16)14(18)19-10-6-4-9(8-17)5-7-10/h1-7
InchiKey:	RJQISSUFUKXVBN-UHFFFAOYSA-N
Formula:	C14H7ClFNO2
SMILES:	N#Cc1ccc(OC(=O)c2cccc(Cl)c2F)cc1
Mol. weight [g/mol]:	275.66

## Physical Properties

Property code	Value	Unit	Source
gf	-44.55	kJ/mol	Joback Method
hf	-185.41	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.570		Crippen Method
mcvol	183.430	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinsol	2258.00		NIST Webbook
tb	803.09	K	Joback Method
tc	1049.78	K	Joback Method
tf	505.60	K	Joback Method
vc	0.721	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.48	J/mol×K	803.09	Joback Method
cpg	467.02	J/mol×K	844.21	Joback Method
cpg	475.61	J/mol×K	885.32	Joback Method
cpg	483.27	J/mol×K	926.44	Joback Method
cpg	490.04	J/mol×K	967.55	Joback Method
cpg	495.95	J/mol×K	1008.67	Joback Method
cpg	501.03	J/mol×K	1049.78	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=U357732&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357732&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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