

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

Inchi:	InChI=1S/C13H6Cl3FO2/c14-9-5-4-7(6-11(9)16)19-13(18)8-2-1-3-10(15)12(8)17/h1-6H
InchiKey:	UQUHAAHZWIDVOX-UHFFFAOYSA-N
Formula:	C13H6Cl3FO2
SMILES:	O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc(Cl)c1F
Mol. weight [g/mol]:	319.54

## Physical Properties

Property code	Value	Unit	Source
gf	-219.64	kJ/mol	Joback Method
hf	-372.60	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.005		Crippen Method
mcvol	192.440	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	757.97	K	Joback Method
tc	1004.92	K	Joback Method
tf	501.70	K	Joback Method
vc	0.737	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.57	J/mol×K	757.97	Joback Method
cpg	445.33	J/mol×K	799.13	Joback Method
cpg	454.17	J/mol×K	840.29	Joback Method
cpg	462.11	J/mol×K	881.45	Joback Method
cpg	469.18	J/mol×K	922.61	Joback Method
cpg	475.40	J/mol×K	963.76	Joback Method
cpg	480.80	J/mol×K	1004.92	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U357733&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357733&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>hvp:</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>rinp:</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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