

# 3-Chloro-2-fluorobenzoic acid, isobutyl ester

<b>Inchi:</b>	InChI=1S/C11H12ClFO2/c1-7(2)6-15-11(14)8-4-3-5-9(12)10(8)13/h3-5,7H,6H2,1-2H3
<b>InchiKey:</b>	GWOJLUGHIBLUHF-UHFFFAOYSA-N
<b>Formula:</b>	C11H12ClFO2
<b>SMILES:</b>	CC(C)COC(=O)c1cccc(Cl)c1F
<b>Mol. weight [g/mol]:</b>	230.66

## Physical Properties

Property code	Value	Unit	Source
gf	-308.21	kJ/mol	Joback Method
hf	-518.71	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.292		Crippen Method
mvol	163.540	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	600.27	K	Joback Method
tc	809.94	K	Joback Method
tf	352.86	K	Joback Method
vc	0.628	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.72	J/mol×K	600.27	Joback Method
cpg	393.46	J/mol×K	635.22	Joback Method
cpg	405.48	J/mol×K	670.16	Joback Method
cpg	416.79	J/mol×K	705.11	Joback Method
cpg	427.40	J/mol×K	740.05	Joback Method
cpg	437.33	J/mol×K	775.00	Joback Method
cpg	446.58	J/mol×K	809.94	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338879&amp;Units=SI</a>
<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>

# 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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