3-Chloro-2-fluorobenzoic acid, butyl ester

Inchi: InChI=1S/C11H12ClFO2/c1-2-3-7-15-11(14)8-5-4-6-9(12)10(8)13/h4-6H,2-3,7H2,1H3
InchiKey: QACRPDSIVSSJJU-UHFFFAOYSA-N
Formula: C11H12ClFO2
SMILES: CCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 230.66

Physical Properties

Property code	Value	Unit	Source
gf	-305.77	kJ/mol	Joback Method
hf	-513.43	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.436		Crippen Method
mcvol	163.540	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
tb	600.71	K	Joback Method
tc	806.23	K	Joback Method
tf	367.86	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.28	J/mol×K	600.71	Joback Method
cpg	392.71	J/mol×K	634.96	Joback Method
cpg	404.47	J/mol×K	669.22	Joback Method
cpg	415.55	J/mol×K	703.47	Joback Method
cpg	425.97	J/mol×K	737.72	Joback Method
cpg	435.75	J/mol×K	771.97	Joback Method
cpg	444.88	J/mol×K	806.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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