3-Chloro-2-fluorobenzoic acid, isopropyl ester

Inchi: InChI=1S/C10H10ClFO2/c1-6(2)14-10(13)7-4-3-5-8(11)9(7)12/h3-6H,1-2H3
InchiKey: HZFZKJTTXAZAHD-UHFFFAOYSA-N
Formula: C10H10ClFO2
SMILES: CC(C)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 216.64

Physical Properties

Property code	Value	Unit	Source
gf	-316.63	kJ/mol	Joback Method
hf	-498.07	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	53.79	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.044		Crippen Method
mcvol	149.450	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1410.00		NIST Webbook
tb	577.39	K	Joback Method
tc	790.54	K	Joback Method
tf	341.59	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.89	J/mol×K	577.39	Joback Method
cpg	345.79	J/mol×K	612.92	Joback Method
cpg	357.03	J/mol×K	648.44	Joback Method
cpg	367.61	J/mol×K	683.97	Joback Method
cpg	377.53	J/mol×K	719.49	Joback Method
cpg	386.81	J/mol×K	755.02	Joback Method
cpg	395.45	J/mol×K	790.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357719&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

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