3-Chloro-2-fluorobenzoic acid, propyl ester

Inchi: InChI=1S/C10H10ClFO2/c1-2-6-14-10(13)7-4-3-5-8(11)9(7)12/h3-5H,2,6H2,1H3
InchiKey: LNXJUYUBVHDCPS-UHFFFAOYSA-N
Formula: C10H10ClFO2
SMILES: CCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 216.64

Physical Properties

Property code	Value	Unit	Source
gf	-314.19	kJ/mol	Joback Method
hf	-492.79	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	54.18	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.046		Crippen Method
mcvol	149.450	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
tb	577.83	K	Joback Method
tc	786.58	K	Joback Method
tf	356.59	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.46	J/mol×K	577.83	Joback Method
cpg	345.07	J/mol×K	612.62	Joback Method
cpg	356.04	J/mol×K	647.41	Joback Method
cpg	366.39	J/mol×K	682.21	Joback Method
cpg	376.12	J/mol×K	717.00	Joback Method
cpg	385.24	J/mol×K	751.79	Joback Method
cpg	393.77	J/mol×K	786.58	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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