3-Chloro-2-fluorobenzoic acid, 2-chloroethyl ester

Inchi: InChI=1S/C9H7Cl2FO2/c10-4-5-14-9(13)6-2-1-3-7(11)8(6)12/h1-3H,4-5H2
InchiKey: RPWPFBWQFNRFTK-UHFFFAOYSA-N
Formula: C9H7Cl2FO2
SMILES: O=C(OCCCl)c1cccc(Cl)c1F
Mol. weight [g/mol]: 237.06

Physical Properties

Property code	Value	Unit	Source
gf	-334.54	kJ/mol	Joback Method
hf	-487.89	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.875		Crippen Method
mcvol	147.600	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	592.38	K	Joback Method
tc	808.67	K	Joback Method
tf	375.24	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.26	J/mol×K	592.38	Joback Method
cpg	321.20	J/mol×K	628.43	Joback Method
cpg	330.53	J/mol×K	664.48	Joback Method
cpg	339.28	J/mol×K	700.53	Joback Method
cpg	347.43	J/mol×K	736.58	Joback Method
cpg	355.02	J/mol×K	772.63	Joback Method
cpg	362.04	J/mol×K	808.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357327&Units=SI

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