3-Chloro-2-fluorobenzoic acid, heptyl ester

Inchi: InChI=1S/C14H18ClFO2/c1-2-3-4-5-6-10-18-14(17)11-8-7-9-12(15)13(11)16/h7-9H,2-6,1
InchiKey: NWJMUVQKIPIXGR-UHFFFAOYSA-N
Formula: C14H18ClFO2
SMILES: CCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 272.74

Physical Properties

Property code	Value	Unit	Source
gf	-280.51	kJ/mol	Joback Method
hf	-575.35	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	63.08	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.606		Crippen Method
mcvol	205.810	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1907.00		NIST Webbook
tb	669.35	K	Joback Method
tc	866.76	K	Joback Method
tf	401.67	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.14	J/mol×K	669.35	Joback Method
cpg	544.46	J/mol×K	702.25	Joback Method
cpg	557.99	J/mol×K	735.15	Joback Method
cpg	570.73	J/mol×K	768.06	Joback Method
cpg	582.71	J/mol×K	800.96	Joback Method
cpg	593.94	J/mol×K	833.86	Joback Method
cpg	604.44	J/mol×K	866.76	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=U338884&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