3-Chloro-2-fluorobenzoic acid, isohexyl ester

Inchi: InChI=1S/C13H16ClFO2/c1-9(2)5-4-8-17-13(16)10-6-3-7-11(14)12(10)15/h3,6-7,9H,4-5,8

InchiKey: XNXMQWMZQFKWNO-UHFFFAOYSA-N

Formula: C13H16ClFO2

SMILES: CC(C)CCCOC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 258.72

Physical Properties

Property code	Value	Unit	Source
gf	-291.37	kJ/mol	Joback Method
hf	-559.99	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	60.47	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.072		Crippen Method
mcvol	191.720	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	646.03	K	Joback Method
tc	849.49	K	Joback Method
tf	375.40	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.19	J/mol×K	646.03	Joback Method
cpg	493.27	J/mol×K	679.94	Joback Method
cpg	506.54	J/mol×K	713.85	Joback Method
cpg	519.02	J/mol×K	747.76	Joback Method
cpg	530.74	J/mol×K	781.67	Joback Method
cpg	541.70	J/mol×K	815.58	Joback Method
cpg	551.92	J/mol×K	849.49	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=U338882&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