3-Chloro-2-fluorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H3ClF6O2/c14-5-3-1-2-4(6(5)15)13(21)22-12-10(19)8(17)7(16)9(18)11(12)
InchiKey: LEMGXRHAERNQBD-UHFFFAOYSA-N
Formula: C13H3ClF6O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1cccc(Cl)c1F
Mol. weight [g/mol]: 340.61

Physical Properties

Property code	Value	Unit	Source
gf	-1198.72	kJ/mol	Joback Method
hf	-1356.08	kJ/mol	Joback Method
hfus	40.25	kJ/mol	Joback Method
hvap	62.36	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.394		Crippen Method
mcvol	176.810	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1686.00		NIST Webbook
tb	694.40	K	Joback Method
tc	892.68	K	Joback Method
tf	482.37	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.21	J/mol×K	694.40	Joback Method
cpg	438.18	J/mol×K	727.45	Joback Method
cpg	446.58	J/mol×K	760.49	Joback Method
cpg	454.38	J/mol×K	793.54	Joback Method
cpg	461.60	J/mol×K	826.59	Joback Method
cpg	468.24	J/mol×K	859.64	Joback Method
cpg	474.29	J/mol×K	892.68	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=U360581&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