3-Chloro-2-fluorobenzoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C11H5ClF8O2/c12-6-3-1-2-5(7(6)13)8(21)22-4-9(14,15)10(16,17)11(18,19)20/

InchiKey: WCFCNXHSTQWYIC-UHFFFAOYSA-N

Formula: C11H5ClF8O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)F)c1cccc(Cl)c1F

Mol. weight [g/mol]: 356.60

Physical Properties

Property code	Value	Unit	Source
gf	-1660.92	kJ/mol	Joback Method
hf	-1912.45	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.469		Crippen Method
mcvol	175.930	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1285.00		NIST Webbook
tb	585.91	K	Joback Method
tc	763.33	K	Joback Method
tf	379.25	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.34	J/mol×K	585.91	Joback Method
cpg	458.75	J/mol×K	615.48	Joback Method
cpg	468.37	J/mol×K	645.05	Joback Method
cpg	477.24	J/mol×K	674.62	Joback Method
cpg	485.41	J/mol×K	704.19	Joback Method
cpg	492.93	J/mol×K	733.76	Joback Method
cpg	499.85	J/mol×K	763.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357325&Units=SI
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

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