

3-Chloro-2-fluorobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H6ClF9O2/c13-6-3-1-2-5(7(6)14)8(23)24-4-10(17,18)12(21,22)11(19,20)9(2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24)
InchiKey: YBSFCAMNTKNDEA-UHFFFAOYSA-N
Formula: C12H6ClF9O2
SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1cccc(Cl)c1F
Mol. weight [g/mol]: 388.61

Physical Properties

Property code	Value	Unit	Source
gf	-1849.75	kJ/mol	Joback Method
hf	-2134.48	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.807		Crippen Method
mcvol	191.790	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	607.62	K	Joback Method
tc	779.99	K	Joback Method
tf	376.11	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.53	J/mol×K	607.62	Joback Method
cpg	515.25	J/mol×K	636.35	Joback Method
cpg	525.18	J/mol×K	665.08	Joback Method
cpg	534.37	J/mol×K	693.80	Joback Method
cpg	542.86	J/mol×K	722.53	Joback Method
cpg	550.70	J/mol×K	751.26	Joback Method
cpg	557.94	J/mol×K	779.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U360578&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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