3-Fluorobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H7F9O2/c13-7-3-1-2-6(4-7)8(22)23-5-10(16,17)12(20,21)11(18,19)9(14)15

InchiKey: YWVCFSSGXHKWPF-UHFFFAOYSA-N

Formula: C12H7F9O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1cccc(F)c1

Mol. weight [g/mol]: 354.17

Physical Properties

Property code	Value	Unit	Source
gf	-1828.19	kJ/mol	Joback Method
hf	-2107.27	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.154		Crippen Method
mcvol	179.550	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1282.00		NIST Webbook
tb	565.21	K	Joback Method
tc	731.87	K	Joback Method
tf	333.67	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.75	J/mol×K	565.21	Joback Method
cpg	489.74	J/mol×K	592.99	Joback Method
cpg	500.89	J/mol×K	620.76	Joback Method
cpg	511.26	J/mol×K	648.54	Joback Method
cpg	520.90	J/mol×K	676.31	Joback Method
cpg	529.83	J/mol×K	704.09	Joback Method
cpg	538.11	J/mol×K	731.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355659&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