4-Fluoro-2-trifluoromethylbenzoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C12H5F11O2/c13-5-1-2-6(7(3-5)10(16,17)18)8(24)25-4-9(14,15)11(19,20)12(2

InchiKey: HWCONUZXSAGTHB-UHFFFAOYSA-N

Formula: C12H5F11O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)F)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 390.15

Physical Properties

Property code	Value	Unit	Source
gf	-2222.16	kJ/mol	Joback Method
hf	-2514.43	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	40.89	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.834		Crippen Method
mcvol	183.090	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	565.94	K	Joback Method
tc	725.76	K	Joback Method
tf	364.79	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.91	J/mol×K	565.94	Joback Method
cpg	508.07	J/mol×K	592.58	Joback Method
cpg	518.41	J/mol×K	619.21	Joback Method
cpg	528.00	J/mol×K	645.85	Joback Method
cpg	536.88	J/mol×K	672.49	Joback Method
cpg	545.08	J/mol×K	699.12	Joback Method
cpg	552.67	J/mol×K	725.76	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=U343764&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