3-Fluoro-4-trifluoromethylbenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C13H6F12O2/c14-7-3-5(1-2-6(7)12(21,22)23)8(26)27-4-10(17,18)13(24,25)11(

InchiKey: JUFNFPARVIHWPA-UHFFFAOYSA-N

Formula: C13H6F12O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 422.17

Physical Properties

Property code	Value	Unit	Source
gf	-2410.99	kJ/mol	Joback Method
hf	-2736.46	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.172		Crippen Method
mcvol	198.950	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	1278.00		NIST Webbook
rinpol	1278.00		NIST Webbook
tb	587.65	K	Joback Method
tc	744.22	K	Joback Method
tf	361.65	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.69	J/mol×K	587.65	Joback Method
cpg	565.08	J/mol×K	613.75	Joback Method
cpg	575.67	J/mol×K	639.84	Joback Method
cpg	585.51	J/mol×K	665.94	Joback Method
cpg	594.65	J/mol×K	692.03	Joback Method
cpg	603.12	J/mol×K	718.13	Joback Method
cpg	610.97	J/mol×K	744.22	Joback Method

Sources

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=U360591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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