9-Oxanonanoic acid, PFBO, methyl ester

Inchi: InChI=1S/C17H20F5NO3/c1-25-12(24)8-6-4-2-3-5-7-9-23-26-10-11-13(18)15(20)17(22)1
InchiKey: KMAWDKLZQXDMIE-NUGSKGIGSA-N
Formula: C17H20F5NO3
SMILES: COC(=O)CCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 381.34

Physical Properties

Property code	Value	Unit	Source
hf	-1490.38	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.788		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	811.68	K	Joback Method
tc	999.04	K	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=R399014&Units=SI

Legend

hf: Enthalpy of formation 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