8-Oxaoctanoic acid, PFBO, methyl ester

Inchi: InChI=1S/C16H18F5NO3/c1-24-11(23)7-5-3-2-4-6-8-22-25-9-10-12(17)14(19)16(21)15(2
InchiKey: XKDMMMKQMCRDJS-UHFFFAOYSA-N
Formula: C16H18F5NO3
SMILES: COC(=O)CCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 367.31

Physical Properties

Property code	Value	Unit	Source
hf	-1469.74	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.398		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	1963.00		NIST Webbook
tb	788.80	K	Joback Method
tc	974.29	K	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=R398937&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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