9,11-Octadecadienoic acid, 13-oxo, PFBO, methyl ester, # 1

Inchi: InChI=1S/C26H34F5NO3/c1-3-4-12-15-19(16-13-10-8-6-5-7-9-11-14-17-21(33)34-2)32-3

InchiKey: AXYWYQNRAHYVEU-NGWPBJGLSA-N

Formula: C26H34F5NO3

SMILES: CCCCCC(C=CC=CCCCCCCCC(=O)OC)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 503.55

Physical Properties

Property code	Value	Unit	Source
hf	-1451.49	kJ/mol	Joback Method
hvap	89.85	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	7.851		Crippen Method
mcvol	372.680	ml/mol	McGowan Method
pc	750.61	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	1025.80	K	Joback Method
tc	1264.39	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=R398942&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