(E)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, «omega»-PFB-oxime

Inchi: InChI=1S/C20H22F5NO4/c1-29-15(28)10-6-4-2-3-5-8-13(27)9-7-11-26-30-12-14-16(21)1

InchiKey: LONGJJDENAGZAX-RXTJIVFLSA-N

Formula: C20H22F5NO4

SMILES: COC(=O)CCCCCCCC(=O)C=CC=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 435.38

Physical Properties

Property code	Value	Unit	Source
hf	-1547.66	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.913		Crippen Method
mcvol	294.010	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	2621.00		NIST Webbook
rinpol	2621.00		NIST Webbook
tb	938.35	K	Joback Method
tc	1148.81	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R554880&Units=SI

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

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