9-Oxo-11-octadecenoic acid, 13-hydroxy, PFBO, TMS, methyl ester, # 1

Inchi: InChI=1S/C29H44F5NO4Si/c1-6-7-11-17-22(39-40(3,4)5)18-14-16-21(15-12-9-8-10-13-1

InchiKey: KBXSLHZIIQGLRI-UJTXETAMSA-N

Formula: C29H44F5NO4Si

SMILES: CCCCCC(C=CCC(CCCCCCCC(=O)OC)=NOCc1c(F)c(F)c(F)c(F)c1F)O[Si](C)(C)C

Mol. weight [g/mol]: 593.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.43		Crippen Method
logp	8.905		Crippen Method
rinpol	2856.00		NIST Webbook
rinpol	2856.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R399029&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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