

9-Oxo-11-octadecenoic acid, 13-hydroxy, PFBO, TMS, methyl ester, # 2

Inchi: InChI=1S/C29H44F5NO4Si/c1-6-7-11-17-22(39-40(3,4)5)18-14-16-21(15-12-9-8-10-13-14)O[Si](C)(C)C
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	2865.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R399034&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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<https://www.chemeo.com/cid/113-796-3/9-Oxo-11-octadecenoic-acid-13-hydroxy-PFBO-TMS-methyl-ester-2.pdf>

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