(E)-10-Dodecenoic acid, 9-hydroxy-12-oxo, methyl ester, MSTFA-adduct, OH-TMS, # 1

Inchi: InChI=1S/C22H42F3NO5Si2/c1-26(21(28)22(23,24)25)19(31-33(6,7)8)17-16-18(30-32(3

InchiKey: JEUZFGKDQQMNDE-WUKNDPDISA-N

Formula: C22H42F3NO5Si2

SMILES: COC(=O)CCCCCCCC(C=CC(O[Si](C)(C)C)N(C)C(=O)C(F)(F)F)O[Si](C)(C)C

Mol. weight [g/mol]: 513.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	5.865		Crippen Method
rinpol	2317.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R554924&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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