12-Oxa-9-dodecenoic acid, 11-hydroxy, PFBO, TMS, methyl ester

Inchi: InChI=1S/C23H32F5NO4Si/c1-31-18(30)13-11-9-7-5-6-8-10-12-16(33-34(2,3)4)14-29-32

InchiKey: RDNFVVMPWOBOFE-ICPIZKTASA-N

Formula: C23H32F5NO4Si

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

Mol. weight [g/mol]: 509.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.91		Crippen Method
logp	6.564		Crippen Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		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=R398828&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices