12-Octadecenoic acid, 11-hydroxy, 9,10-epoxy, TMS, methyl ester, # 3

Inchi: InChI=1S/C22H42O4Si/c1-6-7-8-10-14-17-20(26-27(3,4)5)22-19(25-22)16-13-11-9-12-15

InchiKey: FUHPXBDXDJMGOK-VKAVYKQESA-N

Formula: C22H42O4Si

SMILES: CCCCCC=CC(O[Si](C)(C)C)C1OC1CCCCCCCC(=O)OC

Mol. weight [g/mol]: 398.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	6.014		Crippen Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		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=R398813&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices