

12,13-Epoxy-11-hydroxyoctadec-9-enoic acid, methyl ester, trimethylsilyl ether

Other names: 9-Octadecenoic acid, 11-hydroxy, 12,13-epoxy, TMS, methyl ester, # 2
Inchi: InChI=1S/C22H42O4Si/c1-6-7-13-16-19-22(25-19)20(26-27(3,4)5)17-14-11-9-8-10-12-15
InchiKey: JGPCFZCXXCTAPA-SAPNQHFASA-N
Formula: C22H42O4Si
SMILES: CCCCCC1OC1C(C=CCCCCCCCC(=O)OC)O[Si](C)(C)C
Mol. weight [g/mol]: 398.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	6.014		Crippen Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		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=U368676&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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