

9,10-epoxy-18-hydroxyoctadec-12-enoic acid, methyl ester TMSi ether

Inchi: InChI=1S/C22H42O4Si/c1-24-22(23)18-14-10-7-9-13-17-21-20(26-21)16-12-8-5-6-11-15
InchiKey: RKBGTYUMOJVKKZ-WQLSENKSSA-N
Formula: C22H42O4Si
SMILES: COC(=O)CCCCCCCC1OC1CC=CCCCCO[Si](C)(C)C
Mol. weight [g/mol]: 398.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	6.016		Crippen Method
rinpol	2700.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R423820&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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