

12-Octadecenoic acid, 11-hydroxy, 9,10-epoxy, TMS, methyl ester, # 1

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	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398799&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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