

12-Octadecenoic acid, 11-hydroxy, 9,10-epoxy, TMS, methyl ester, #2

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)C1OC1CCCCCCCCC(=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	2408.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398808&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/66-633-6/12-Octadecenoic-acid-11-hydroxy-9-10-epoxy-TMS-methyl-ester-2.pdf>

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