

Octadecanoic acid, 9,10-epoxy-18-(trimethylsiloxy)-, methyl ester, cis-

Other names:

9,10-epoxy-18-hydroxyoctadecanoic acid, methyl ester TMSi ether

Inchi:

InChI=1S/C22H44O4Si/c1-24-22(23)18-14-10-7-9-13-17-21-20(26-21)16-12-8-5-6-11-15

InchiKey:

CEOPGRLHKCOWTE-LEWJYISDSA-N

Formula:

C22H44O4Si

SMILES:

COC(=O)CCCCCCCC1OC1CCCCCCCCO[Si](C)(C)C

Mol. weight [g/mol]:

400.67

CAS:

22032-78-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	6.240		Crippen Method
rinpol	2731.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C22032786&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/84-404-0/Octadecanoic-acid-9-10-epoxy-18-trimethylsiloxy-methyl-ester-cis.pdf>

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