

Hexadecanoic acid, 10,16-bis[(trimethylsilyl)oxy]-, methyl ester

Other names:

Hexadecanoic acid, 10,16-bis(trimethylsiloxy)-, methyl ester

10,16-dihydroxyhexadecanoic acid, methyl ester TMSi ether

Inchi:

InChI=1S/C23H50O4Si2/c1-25-23(24)20-16-11-9-8-10-14-18-22(27-29(5,6)7)19-15-12-1

InchiKey:

LSNBUNAPGUZSSF-UHFFFAOYSA-N

Formula:

C23H50O4Si2

SMILES:

COC(=O)CCCCCCCC(CCCCCO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]:

446.81

CAS:

21987-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	7.302		Crippen Method
rinpol	2470.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2460.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C21987166&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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