Hexadecanoic acid, 2,3-bis[(trimethylsilyl)oxy]propyl ester

Other names: 1-Monopalmitin trimethylsilyl ether
1-Monopalmitoylglycerol trimethylsilyl ether
Hexadecanoic acid, 2,3-bis-(OTMS) propyl ester («alpha»-glyceryl palmitate)
monopalmitin TMS
«alpha»-Glyceryl palmitate, bis-TMS
«alpha»-Glyceryl palmitate, di-TMS
1-Monopalmitin, 2tms derivative

Inchi: InChI=1S/C25H54O4Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25(26)27-22-24(2

InchiKey: LUHPQMTVPLRAQA-UHFFFAOYSA-N

Formula: C25H54O4Si2

SMILES: CCCCCCCCCCCCCCCC(=O)OCC(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 474.86

CAS: 1188-74-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	8.082		Crippen Method
rinpol	2574.10		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2607.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2611.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2574.10		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1188745&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