

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

Other names:

Eicosanoic acid, 2,3-bis-(OTMS)propyl ester
1-Glycerol, mono-eicosanoate, bis-(O-TMS)-
Arachidic acid, 2,3-bis[(trimethylsilyl)oxy]propyl ester
«alpha»-Glycerol arachidate, bis-(O-TMS)-
Eicosanoic acid, 2,3-bis-(OTMS) propyl ester («alpha»-glycerol arachidate)
«alpha»-Glycerol eicosanoate, TMS
Glycerol, mono-eicosanoate, bis-TMS
2,3-Dihydroxypropyl icosanoate, 2tms derivative

Inchi: InChI=1S/C29H62O4Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-29(3

InchiKey: KIQRTLCOMLAEFH-UHFFFAOYSA-N

Formula: C29H62O4Si2

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

Mol. weight [g/mol]: 530.97

CAS: 55517-94-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	9.643		Crippen Method
rinpol	2960.10		NIST Webbook
rinpol	2998.00		NIST Webbook
rinpol	2999.00		NIST Webbook
rinpol	3000.00		NIST Webbook
rinpol	2960.10		NIST Webbook
rinpol	2999.00		NIST Webbook
rinpol	2998.00		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517947&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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