

Eicosanoic acid, 2-[(trimethylsilyl)oxy]-1-[[trimethylsilyl]oxy]methyl ester

Other names:	Eicosanoic acid, 1,3-bis-(OTMS) propyl ester («beta»-glyceryl arachidate)
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:	KCRAQFLKPNSNSO-UHFFFAOYSA-N
Formula:	C29H62O4Si2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OC(CO[Si](C)(C)C)CO[Si](C)(C)C
Mol. weight [g/mol]:	530.97
CAS:	55517-93-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	9.643		Crippen Method
rinpol	2965.00		NIST Webbook
rinpol	2962.00		NIST Webbook
rinpol	2965.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/124-974-3/Eicosanoic-acid-2-trimethylsilyl-oxy-1-trimethylsilyl-oxy-methyl-ethyl-ester.pdf>

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