

Octadecanoic acid, 12-(trimethylsiloxy)-, trimethylsilyl ester

Other names:	Trimethylsilyl (12-trimethylsiloxy)stearate 12-Hydroxystearic acid, TMS
Inchi:	InChI=1S/C24H52O3Si2/c1-8-9-10-17-20-23(26-28(2,3)4)21-18-15-13-11-12-14-16-19-2
InchiKey:	JVAFKRMVDNBHPD-UHFFFAOYSA-N
Formula:	C24H52O3Si2
SMILES:	CCCCCCC(CCCCCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	444.84
CAS:	22396-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	8.456		Crippen Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22396221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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