

1,14-Tetradecandioic acid , bis(trimethylsilyl) ester

Other names:	1,14-Tetradecandioic acid, di-TMS Tetradecanedioic acid, bis-TMS Tetradecanedioic acid, bis(trimethylsilyl) ester Tetradecanedioic acid, 2tms derivative
Inchi:	InChI=1S/C20H42O4Si2/c1-25(2,3)23-19(21)17-15-13-11-9-7-8-10-12-14-16-18-20(22)2
InchiKey:	OCCHGMDNQHG UHB-UHFFFAOYSA-N
Formula:	C20H42O4Si2
SMILES:	C[Si](C)(C)OC(=O)CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	402.72
CAS:	139432-41-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	6.424		Crippen Method
rmpol	2277.00		NIST Webbook
rmpol	2269.00		NIST Webbook
rmpol	2277.00		NIST Webbook
rmpol	2305.00		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=C139432410&Units=SI

Legend

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

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