

Hexanedioic acid, 2-trimethylsilyloxy-, bis(trimethylsilyl) ester

Other names:	2,3,4-Trideoxyhexaric acid, TMS 2-Hydroxyadipic acid, triTMS
Inchi:	InChI=1S/C15H34O5Si3/c1-21(2,3)18-13(15(17)20-23(7,8)9)11-10-12-14(16)19-22(4,5)6
InchiKey:	SCMUEAPKCNESSEW-UHFFFAOYSA-N
Formula:	C15H34O5Si3
SMILES:	C[Si](C)(C)OC(=O)CCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	378.68

Physical Properties

Property code	Value	Unit	Source
log10ws	2.82		Crippen Method
logp	4.133		Crippen Method
rinpol	1689.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1679.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U71969&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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