

3-Hydroxyoctanoic acid, di-TMS

Other names:	Octanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester
Inchi:	InChI=1S/C14H32O3Si2/c1-8-9-10-11-13(16-18(2,3)4)12-14(15)17-19(5,6)7/h13H,8-12H
InchiKey:	CVUFVRMCXZJNTH-UHFFFAOYSA-N
Formula:	C14H32O3Si2
SMILES:	CCCCC(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	304.57
CAS:	141-42-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	4.555		Crippen Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		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=C141424&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-354-5/3-Hydroxyoctanoic-acid-di-TMS.pdf>

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