

2,4-Dodeoxy-3-C-methylpentonic acid, tris-TMS

Inchi:	InChI=1S/C15H36O4Si3/c1-15(19-22(8,9)10,11-12-17-20(2,3)4)13-14(16)18-21(5,6)7/h1
InchiKey:	HUAKLDAFGDRXAP-UHFFFAOYSA-N
Formula:	C15H36O4Si3
SMILES:	CC(CCO[Si](C)(C)C)(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	364.70

Physical Properties

Property code	Value	Unit	Source
log10ws	2.60		Crippen Method
logp	4.606		Crippen Method
rinpol	1575.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R100735&Units=SI

Legend

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

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