

12-«beta»-Hydroxy-GA13, methyl ester, TMS

Inchi:	InChI=1S/C29H48O8Si2/c1-17-15-28-16-18(17)19(36-38(6,7)8)14-20(28)29(26(32)35-5)
InchiKey:	SLGPATXYODBIAO-OGHXHMLQSA-N
Formula:	C29H48O8Si2
SMILES:	<chem>C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)OC)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1</chem>
Mol. weight [g/mol]:	580.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	4.951		Crippen Method
rinpol	2791.00		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=R388539&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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