

16«beta»,17-H2(OH)2 GA12, MeTMSi

Other names:	16«beta»,17-di-(OH)-16,17-dihydroGA12, Me-TMS
Inchi:	InChI=1S/C28H50O6Si2/c1-25-14-11-15-26(2,24(30)32-4)22(25)21(23(29)31-3)27-16-19
InchiKey:	ZZFWQNAQASSFEN-QPJDJCVSA-N
Formula:	C28H50O6Si2
SMILES:	COC(=O)C1C2C(C)(C(=O)OC)CCCC2(C)C2CCC3CC12CC3(CO[Si](C)(C)C)O[Si](C)(C)
Mol. weight [g/mol]:	538.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	6.023		Crippen Method
rinpola	2748.00		NIST Webbook
rinpola	2750.00		NIST Webbook
rinpola	2741.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258463&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-190-4/16-beta-17-H2-OH-2-GA12-MeTMSi.pdf>

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