

16«alpha»,17-H2(OH)2 GA12, MeTMSi

Other names: 16«alpha», 17-H2 (OH)2 GA12, MeTMS
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-WIEZBTDDSA-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
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2780.00		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=R258423&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/67-182-6/16-alpha-17-H2-OH-2-GA12-MeTMSi.pdf>

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