

[13C] 16«alpha», 17-H2-16, 17-(OH)2-GA4 methyl ester TMS ether

Other names: 16«alpha»,17-H2 (OH)2 GA4, MeTMS
Inchi: InChI=1S/C29H52O7Si3/c1-26-21(35-38(6,7)8)14-15-29(34-25(26)31)20-13-12-19-16-27
InchiKey: KTOFHXXWALBMWHS-GZKFZNCGSA-N
Formula: C29H52O7Si3
SMILES: COC(=O)C1C2C3(CCC(O[Si](C)(C)C)C2(C)C(=O)O3)C2CCC3CC12CC3(CO[Si](C)(C)C)C
Mol. weight [g/mol]: 596.98

Physical Properties

Property code	Value	Unit	Source
log10ws	0.54		Crippen Method
logp	5.969		Crippen Method
rinpol	2926.00		NIST Webbook
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
rinpol	2925.00		NIST Webbook
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
rinpol	2891.00		NIST Webbook
rinpol	2932.00		NIST Webbook
rinpol	2923.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R176811&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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