

16«alpha»,17-H2(OH)2-GA7, MeTMS

Inchi: InChI=1S/C29H50O7Si3/c1-26-21(35-38(6,7)8)14-15-29(34-25(26)31)20-13-12-19-16-27
InchiKey: MLWPTDHDQIZUITI-GZKFZNCGSA-N
Formula: C29H50O7Si3
SMILES: COC(=O)C1C2C3(C=CC(O[Si](C)(C)C)C2(C)C(=O)O3)C2CCC3CC12CC3(CO[Si](C)(C)C)C3
Mol. weight [g/mol]: 594.96

Physical Properties

Property code	Value	Unit	Source
log10ws	0.69		Crippen Method
logp	5.745		Crippen Method
rinpol	2947.00		NIST Webbook
rinpol	2948.00		NIST Webbook
rinpol	2957.00		NIST Webbook
rinpol	2947.00		NIST Webbook
rinpol	2957.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R259906&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-201-5/16-alpha-17-H2-OH-2-GA7-MeTMS.pdf>

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