

16«alpha»,17-H2(OH)2 GA7, MeTMSi

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-JJMHPHSYSA-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	2947.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258443&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/39-622-8/16-alpha-17-H2-OH-2-GA7-MeTMSi.pdf>

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