

17-OH-16«beta»,17-H2 GA53 methyl ester TMS ether

Other names: 16«beta», 17-H2-OH GA53, methyl ester TMS ether
Inchi: InChI=1S/C28H50O6Si2/c1-25-13-11-14-26(2,24(30)32-4)22(25)21(23(29)31-3)27-16-19
InchiKey: IBWSUNLYMOKQBR-UGSMSOJMSA-N
Formula: C28H50O6Si2
SMILES: COC(=O)C1C2C(C)(C(=O)OC)CCCC2(C)C2CCC3(O[Si](C)(C)C)CC12CC3CO[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	2762.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2747.00		NIST Webbook
rinpol	2748.00		NIST Webbook
rinpol	2755.00		NIST Webbook
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
rinpol	2757.00		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=R181269&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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