2«beta»-OH-GA28, methyl ester TMS ether

Inchi: InChI=1S/C32H56O9Si3/c1-20-17-30-19-31(20,41-44(12,13)14)16-15-22(30)32(28(35)38
InchiKey: QKGPRFODNKTFCN-VXXSLBNJSA-N
Formula: C32H56O9Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C1(C(=O)OC)CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)
Mol. weight [g/mol]: 669.04

Physical Properties

Property code	Value	Unit	Source
logp	5.925		Crippen Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177092&Units=SI

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices