12-«alpha»-Hydroxy-GA12, methyl ester, TMS

Inchi: InChI=1S/C25H40O5Si/c1-15-13-25-14-16(15)17(30-31(6,7)8)12-18(25)23(2)10-9-11-24
InchiKey: FQADVUVPWOUFKJ-PHHHHLQSSA-N
Formula: C25H40O5Si
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 448.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	4.967		Crippen Method
rinpol	2538.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R388480&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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