12-«alpha»-Hydroxy-GA5, MeTMSi

Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-26(16,32-34(7,8)9)18(31-33(4,5)6)13-17(24)25-
InchiKey: KQGUPRWOMUWGHL-WFMOHTBYSA-N
Formula: C26H40O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)
Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2641.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R79042&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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