ent-6-«alpha»,7-«alpha»,12-«alpha»-Trihydroxyka
acid, methyl ester, TMS

Inchi: InChI=1S/C30H56O5Si3/c1-20-18-30-19-21(20)22(33-36(5,6)7)17-23(30)28(2)15-14-16-
InchiKey: QBWCWXKMXXCFDO-OFDKGRPOSA-N
Formula: C30H56O5Si3
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCCC(C)(C(=O)OC)C1C(O[Si](C)(C)C)C3O[S
Mol. weight [g/mol]: 581.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	7.619		Crippen Method
rinpol	2769.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R388584&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