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

Inchi: InChI=1S/C27H48O4Si2/c1-18-16-27-17-19(18)20(30-32(5,6)7)14-22(27)25(2)12-11-13-
InchiKey: ABDYOZCWUFZSJY-QPLDEJNASA-N
Formula: C27H48O4Si2
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCCC(C)(C(=O)OC)C1CC3O[Si](C)(C)C
Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	6.788		Crippen Method
rinpol	2615.00		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=R388608&Units=SI

Legend

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