7-«alpha»,12-«alpha»-Dihydroxykaurenolide, TMS

Inchi: InChI=1S/C26H44O4Si2/c1-16-14-26-15-17(16)18(29-31(4,5)6)13-19(26)24(2)11-10-12-

InchiKey: JEBXORPJLHQEOW-POWTWRCSSA-N

Formula: C26H44O4Si2

SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCCC2(C)C(=O)OC(C21)C3O[Si](C)(C)C

Mol. weight [g/mol]: 476.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	6.151		Crippen Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R388564&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