ent-16«beta»,17-H2(OH)2 7«alpha»-OH kaurenoic acid, MeTMSi

Inchi: InChI=1S/C30H58O5Si3/c1-27-16-13-17-28(2,26(31)32-3)24(27)18-25(34-37(7,8)9)29-19

InchiKey: DMPXXORFQWDRPX-OBTUAGNVSA-N

Formula: C30H58O5Si3

SMILES: COC(=O)C1(C)CCCC2(C)C1CC(O[Si](C)(C)C)C13CC(CCC21)C(CO[Si](C)(C)C)(O[Si](C

Mol. weight [g/mol]: 583.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	7.844		Crippen Method
rinpol	2866.00		NIST Webbook
rinpol	2866.00		NIST Webbook
rinpol	2866.00		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=R258507&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices