

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)29-1
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)(C)C)C1
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
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rinpol	2866.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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