

ent-6«alpha»,7«alpha»,17-tri-(OH)-16«beta»,17-dihydrokaurenonic acid, Me-TMS

Inchi: InChI=1S/C30H58O5Si3/c1-28-16-13-17-29(2,27(31)32-3)25(28)24(34-37(7,8)9)26(35-38)30-33-22-21-20-19-18-15-14-12-11-10-9-8-7-6-5-4-3-2-1
InchiKey: MTNGRFRKLJEUIT-JKLCFUQKSA-N

Formula: C30H58O5Si3
SMILES: COC(=O)C1(C)CCCC2(C)C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C13CC(CCC21)C(CO[Si](C)(C)C)C1
Mol. weight [g/mol]: 583.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	7.700		Crippen Method
rinpol	2841.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536926&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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