

7«beta»,16«beta»,17-triOH-kauranolide, TMS

Inchi: InChI=1S/C29H54O5Si3/c1-26-15-12-16-27(2)23(26)22(32-25(27)30)24(33-36(6,7)8)28-
InchiKey: JQOXUXMAXUVRFF-SMASEPDESA-N
Formula: C29H54O5Si3
SMILES: CC12CCCC3(C)C1C(OC2=O)C(O[Si](C)(C)C)C12CC(CCC31)C(CO[Si](C)(C)C)(O[Si](C)(C)C)C12
Mol. weight [g/mol]: 566.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	7.206		Crippen Method
rinpol	3041.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151872&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

Latest version available from:

<https://www.chemeo.com/cid/19-132-4/7-beta-16-beta-17-triOH-kauranolide-TMS.pdf>

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