

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

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-KZOKFAESSA-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
Mol. weight [g/mol]:	566.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	7.206		Crippen Method
rinpol	2896.00		NIST Webbook
rinpol	2898.00		NIST Webbook
rinpol	2896.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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