

7-«alpha»,12-«alpha»-Dihydroxykaurenolide, TMS

Inchi:	InChI=1S/C26H44O4Si2/c1-16-14-26-15-17(16)18(29-31(4,5)6)13-19(26)24(2)11-10-12-
InchiKey:	JEBXORPJLHQEOW-POWTWRCSSA-N
Formula:	C26H44O4Si2
SMILES:	C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCCC2(C)C(=O)OC(C21)C3O[Si](C)(C)C
Mol. weight [g/mol]:	476.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	6.151		Crippen Method
rinpol	2671.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R388564&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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<https://www.cheméo.com/cid/42-133-7/7-alpha-12-alpha-Dihydroxykaurenolide-TMS.pdf>

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