

7-«beta»,12-«beta»-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-FUNFIWAMSA-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	2682.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R388579&Units=SI>

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/66-111-5/7-beta-12-beta-Dihydroxykaurenolide-TMS.pdf>

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