2-«alpha»-Hydroxy-9,15-cyclo-GA9, methyl ester [D2], TMS

Inchi: InChI=1S/C23H32O5Si/c1-12-13-7-8-22-16(12)21(22,9-13)15(18(24)26-3)17-20(2)10-14

InchiKey: JLZFFKANKJYMMT-SKLKLVQMSA-N

Formula: C23H32O5Si

SMILES: C=C1C2CCC34C1C3(C2)C(C(=O)OC)C1C2(C)CC(O[Si](C)(C)C)CC14OC2=O

Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	3.694		Crippen Method
rinpol	2466.00		NIST Webbook
rinpol	2471.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R499793&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/27-544-8/2-alpha-Hydroxy-9-15-cyclo-GA9-methyl-ester-D2-TMS.pdf

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