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

Inchi: InChI=1S/C23H32O5Si/c1-12-13-10-21-15(18(24)26-3)17-20(2)8-7-9-23(17,27-19(20)25)
InchiKey: SQUXDBJNUQQKAQ-SKLKLVQMSA-N
Formula: C23H32O5Si
SMILES: C=C1C2CC34C(C(=O)OC)C5C6(C)CCCC5(OC6=O)C3(CC2O[Si](C)(C)C)C14
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
logp	3.694		Crippen Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R499773&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices