

12-«beta»-Hydroxy-GA14, methyl ester, TMS

Inchi: InChI=1S/C28H48O6Si2/c1-17-15-28-16-18(17)19(33-35(6,7)8)14-20(28)26(2)13-12-21(12)
InchiKey: RUQHTXLJSAGIIL-ZNIXGMTDSA-N
Formula: C28H48O6Si2
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)OC1
Mol. weight [g/mol]: 536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	5.797		Crippen Method
rinpol	2707.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R388544&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

Latest version available from:

<https://www.cheméo.com/cid/55-147-8/12-beta-Hydroxy-GA14-methyl-ester-TMS.pdf>

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