

15-«beta»-Hydroxy-GA3, MeTMSi

Inchi: InChI=1S/C29H48O7Si3/c1-18-23(35-38(7,8)9)28-17-27(18,36-39(10,11)12)15-13-19(28)
InchiKey: ANNVQJIKEDDKCR-GOKBTLLCSA-N
Formula: C29H48O7Si3
SMILES: C=C1C(O[Si](C)(C)C)C23CC1(O[Si](C)(C)C)CCC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O)C
Mol. weight [g/mol]: 592.94

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	5.664		Crippen Method
rinpol	2814.00		NIST Webbook

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=R79109&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/18-837-3/15-beta-Hydroxy-GA3-MeTMSi.pdf>

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