

12-«beta»-Hydroxy-GA3, MeTMSi

Inchi: InChI=1S/C29H48O7Si3/c1-18-16-27-17-29(18,36-39(10,11)12)21(35-38(7,8)9)15-19(27)
InchiKey: CODGHIRYLJNHPK-BAEQSZASSA-N
Formula: C29H48O7Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C12C=CC(O[Si](C)(C)C)C(C)(C(=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	2843.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79074&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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