

12-«beta»-Hydroxy-GA36, methyl ester, TMS

Inchi: InChI=1S/C28H46O7Si2/c1-17-14-28-15-18(17)19(34-36(5,6)7)13-20(28)27(16-29)12-11
InchiKey: FUMVTFXLMVFXIE-PWZATHTESA-N
Formula: C28H46O7Si2
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C=O)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C
Mol. weight [g/mol]: 550.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	4.976		Crippen Method
rinpol	2786.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R388559&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/29-184-6/12-beta-Hydroxy-GA36-methyl-ester-TMS.pdf>

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