

12«beta»-OH-GA9 methyl ester TMS ether

Other names: [13C]GA69, MeTMS
Inchi: InChI=1S/C23H34O5Si/c1-13-11-22-12-14(13)15(28-29(4,5)6)10-16(22)23-9-7-8-21(2,20)
InchiKey: KKEMDAAVLAIFTB-XXMNCVSDSA-N
Formula: C23H34O5Si
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CCCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 418.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	4.084		Crippen Method
rinpol	2493.00		NIST Webbook
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook
rinpol	2493.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151778&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

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<https://www.cheméo.com/cid/70-444-1/12-beta-OH-GA9-methyl-ester-TMS-ether.pdf>

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