

GA70, MeTMS

Other names: 12-«alpha»-Hydroxy-GA9, methyl ester, TMS
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-FNXSURMMSA-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	2549.00		NIST Webbook
rinpol	2561.00		NIST Webbook
rinpol	2541.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2542.00		NIST Webbook
rinpol	2549.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79864&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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/24-150-8/GA70-MeTMS.pdf>

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