

3«alpha»-hydroxy-9,15-cyclo-GA9 (GA107), MeTMS

Inchi:	InChI=1S/C23H32O5Si/c1-12-13-7-9-22-16(12)21(22,11-13)15(18(24)26-3)17-20(2)14(2)
InchiKey:	DJWIPOWTBQNJHO-XIYYVQIMSA-N
Formula:	C23H32O5Si
SMILES:	C=C1C2CCC34C1C3(C2)C(C(=O)OC)C1C2(C)C(=O)OC14CCC2O[Si](C)(C)C
Mol. weight [g/mol]:	416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	3.694		Crippen Method
rinpol	2545.00		NIST Webbook
rinpol	2550.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/30-821-6/3-alpha-hydroxy-9-15-cyclo-GA9-GA107-MeTMS.pdf>

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