

1 «beta»-hydroxy-9,15-cyclo-GA9 (GA104), MeTMS

Inchi:	InChI=1S/C23H32O5Si/c1-12-13-7-10-22-16(12)21(22,11-13)15(18(24)26-3)17-20(2)9-8
InchiKey:	AZSIYLVDBHSVHD-ZMNXUOQGS A-N
Formula:	C23H32O5Si
SMILES:	C=C1C2CCC34C1C3(C2)C(C(=O)OC)C1C2(C)CCC(O[Si](C)(C)C)C14OC2=O
Mol. weight [g/mol]:	416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	3.694		Crippen Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224227&Units=SI

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/44-140-7/1-beta-hydroxy-9-15-cyclo-GA9-GA104-MeTMS.pdf>

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