

12«alpha»-HydroxyGA25, methyl ester TMS

Inchi:	InChI=1S/C26H40O7Si/c1-15-13-25-14-16(15)17(33-34(6,7)8)12-18(25)26(23(29)32-5)1
InchiKey:	HBURFWRACQFAAJ-RJWOBXGISA-N
Formula:	C26H40O7Si
SMILES:	C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)OC)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]:	492.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	4.121		Crippen Method
rinpol	2664.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258750&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/39-266-4/12-alpha-HydroxyGA25-methyl-ester-TMS.pdf>

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