

Androst-5-ene-3«beta»,17«beta»-diol-16-one, TMS

Inchi:	InChI=1S/C28H52O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28
InchiKey:	XHAVWCXDWBVKJK-MQYOSBKTSA-N
Formula:	C28H52O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)=C(O[Si](C)(C)C)CC12
Mol. weight [g/mol]:	520.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	8.694		Crippen Method
rinpol	2760.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R305272&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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