5-Androsten-3««beta»-»ol-17-one, TMS

Inchi:	InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	VEYGGCOAFMQLPU-UNVOLWNJSA-N
Formula:	C25H44O2Si2
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12
Mol. weight [g/mol]:	432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	7.515		Crippen Method
rinpol	2521.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R529463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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https://www.chemeo.com/cid/46-754-4/5-Androsten-3-beta-ol-17-one-TMS.pdf

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