3A-Hydroxy-5B-androstan-17-one, bis-TMS

Other names:	Ethiocholanolone, TMS
	Etiocholanolone, di-TMS
Inchi:	InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	WRVSWIFKEWFLRU-SSIUMMFWSA-N
Formula:	C25H46O2Si2
SMILES:	CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]:	434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	7.594		Crippen Method
rinpol	2543.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2534.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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