

5«alpha»-Androstan-17-one, 3«alpha»,11«beta»-bis(trimethylsiloxy)-

Other names:	3,11-Bis[(trimethylsilyl)oxy]androstan-17-one, (3«alpha»,5«alpha»,11«beta»)-11«beta»-Hydroxyandrosterone, di-TMS 3«alpha»,11«beta»-Dihydroxy-5«alpha»-androstan-17-one, bis-TMS 11B-Hydroxyandrosterone, TMS 3A,11B-Dihydroxy-5A-androstan-17-one, enol, bis-TMS 11-Hydroxyetiocholanolone (3«alpha»,5«alpha»,11«beta»)-, 2tms derivative
Inchi:	InChI=1S/C25H46O3Si2/c1-24-14-13-18(27-29(3,4)5)15-17(24)9-10-19-20-11-12-22(26)
InchiKey:	SVZGBEADGIZYEM-MDUJESLESA-N
Formula:	C25H46O3Si2
SMILES:	CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	450.80
CAS:	17562-92-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	6.648		Crippen Method
rinpol	2681.00		NIST Webbook
rinpol	2693.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17562924&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

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