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

Other names: 3,11-Bis[(trimethylsilyl)oxy]androstan-17-one, (3«alpha»,5«beta»,11«beta»)-
11«beta»-Hydroxyetiocholanolone, bis-TMS
3«alpha»,11«beta»-Dihydroxy-5«beta»-androstan-17-one, bis-TMS
3A,11B-dihydroxy-5B-androstan-17-one, enol, bis-TMS
11B-Hydroxyetiocholanolone, TMS
11-Hydroxyetiocholanolone (3«alpha»,5«beta»,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-WVUMPWGQSA-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: 17562-89-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	6.648		Crippen Method
rinpol	2683.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2693.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17562899&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