3«alpha»,17«beta»-Bis(trimethylsilyloxy)-5«beta»-

Other names:	Silane, [[(3«alpha»,5«beta»,17«beta»)-androstane-3,17-diyl]bis(oxy)bis[-trimethyl- Silane, (5«beta»-androstan-3«alpha»,17«beta»-ylenedioxy)bis[trimethyl- 3,17-Bis[(trimethylsilyl)oxy]androstane, (3«alpha»,5«beta»,17«beta»)- 5-«beta»-Androstan-3-«alpha»,17-«beta»-diol, bis-TMS 5«beta»-Androstanediol-3«alpha»,17«beta», bis-TMS 5beta-Androstan-3alpha,17beta-diol, bis-TMS 5-«beta»-Androstan-3-«alpha»,17-«beta»-diol, TMS 5B-Androstan-3A,17B-diol, bis-TMS 5B-Androstane-3A,17B-diol, TMS Androstane-3,17-diol, (3«alpha»,5«beta»,17«beta»)-, 2tms derivative
Inchi:	InChI=1S/C25H48O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	KBSHKNYEUGMMDQ-ZUHJIWNMSA-N
Formula:	C25H48O2Si2
SMILES:	CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	436.82
CAS:	13111-26-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	7.469		Crippen Method
rinpol	2558.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2581.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2567.00		NIST Webbook
rinpol	2570.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13111267&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices