3«beta»,16«beta»,17«beta»-Tris(trimethylsiloxy)an

Other names:	Silane, [[(3«beta»,16«beta»,17«beta»)-androst-5-ene-3,16,17-triyl]tris(oxy)]tris[trimethyl- Silane, (androst-5-ene-3«beta»,16«beta»,17«beta»-triyltrioxy)tris[trimethyl- Silane, [[(3«beta»,16«beta»,17«beta»)-androst-5-ene-3,16,17-triyl]tris(oxy)]tris*trimethyl- Silane, (androst-5-ene-3«beta»,16«beta»,17«beta»-triyltrioxy)tris*trimethyl- 5-Androsten-3-«beta»,16-«beta»,17-«beta»-triol, TMS
Inchi:	InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28
InchiKey:	HVNNEDKUOOQWAG-FDGJOUIBSA-N
Formula:	C28H54O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]:	522.98
CAS:	33287-31-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	8.219		Crippen Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33287319&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

Latest version available from:

https://www.chemeo.com/cid/71-642-0/3-beta-16-beta-17-beta-Tris-trimethylsiloxy-androst-5-ene.pdf

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