

3«beta»,17,21«alpha»-Tris(trimethylsiloxy)pregn-5

Other names:	Silane, [[(3«beta»,20S)-preg-5-ene-3,17,20-triyl]tris(oxy)]tris(trimethyl- Silane, [[(3«beta»,20S)-preg-5-ene-3,17,20-triyl]tris(oxy)]tris*trimethyl- Tris(trimethylsilyl)- 5-Pregnene-3«beta»,17«alpha»,20«alpha»-triol 5-pregnene-3«beta»,17,20«alpha»-triol, MO-TMS
Inchi:	InChI=1S/C30H58O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21
InchiKey:	LKYVWFBNWTZFW-UHFFFAOYSA-N
Formula:	C30H58O3Si3
SMILES:	CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21
Mol. weight [g/mol]:	551.04
CAS:	41164-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	9.000		Crippen Method
rincpol	2944.00		NIST Webbook
rincpol	2966.00		NIST Webbook
rincpol	2966.00		NIST Webbook
rincpol	2944.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41164196&Units=SI

Legend

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

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