

Silane, [[(3«beta»,20S)-pregn-5-ene-3,20-diol]bis(oxy)]bis

Other names:

Silane, (pregn-5-en-3«beta»,20«alpha»-ylenedioxy)bis[trimethyl-
Pregnane, trimethylsilane deriv.

bis-3«beta»,20«alpha»-Trimethylsilyloxy-5-pregnene

3,20-Bis[(trimethylsilyl)oxy]pregn-5-ene, (3«beta»,20«alpha»)-

5-Pregnen-3«beta»,20«alpha»-diol, bis-TMS

5-Pregnen-3-«beta»,20-«alpha»-diol, TMS

Pregn-5-ene-3,20-diol, (3«beta»,20s)-, 2tms derivative

Inchi: InChI=1S/C27H50O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)

InchiKey: PXQKWROLXRMAD-UHFFFAOYSA-N

Formula: C27H50O2Si2

SMILES: CC(O[Si](C)(C)C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 462.86

CAS: 13110-77-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	8.026		Crippen Method
rinpol	2831.00		NIST Webbook
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
rinpol	2831.00		NIST Webbook
rinpol	2828.00		NIST Webbook
rinpol	2874.00		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=C13110775&Units=SI>

Legend

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

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