

Silane, [(3«alpha»,5«beta»,20S)-pregnane-3,20-diyl]bis(o

Other names:	Silane, (5«beta»-pregnan-3«alpha»,20«alpha»-ylenedioxy)bis[trimethyl- Silane, [(3«alpha»,5«beta»,20«alpha»)-pregnane-3,20-diylbis(oxy)]bis[trimethyl- 3«alpha»,20«alpha»-Bis[(trimethylsilyl)oxy]-5«beta»-pregnane 5«beta»-Pregnane-3«alpha»,20«alpha»-diol, bis(trimethylsilyl) ether 3«alpha»,20«alpha»-Dihydroxy-5«beta»-pregnane, bis-TMS 5«beta»-Pregnane-3«alpha»,20«alpha»-diol, di-TMS Pregnanediol, bis-TMS Pregnanediol, (2TMS) Pregnanediol, TMS 5«beta»-Pregnane-3«alpha»,20«alpha»-diol, TMS 3A,20A-Dihydroxy-5B-pregnane, bis-TMS Pregnane-3,20-diol, (3«alpha»,5«beta»,20s)-, 2tms derivative
Inchi:	InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)
InchiKey:	PSZRAFDARWUCMW-UHFFFAOYSA-N
Formula:	C27H52O2Si2
SMILES:	CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	464.87
CAS:	16134-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2744.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2806.00		NIST Webbook
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
rinpol	2787.00		NIST Webbook
rinpol	2803.90		NIST Webbook
rinpol	2794.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16134568&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

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