

Bis(trimethylsilyl)derivative of 3«beta»,20«beta»-dihydroxypregn-5-ene

Other names:

Silane, [[[3«beta»,20R)-pregn-5-ene-3,20-diyl]bis(oxy)]bis[trimethyl-
Silane, (pregn-5-en-3«beta»,20«beta»-ylenedioxy)bis[trimethyl-
Pregnane, silane deriv.

Bis-3«beta»,20«beta»-trimethylsilyloxy-5-pregnene

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

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

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

Pregn-5-ene-3,20-diol, (3«beta»,20r)-, 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: PXQKWIROLXRMAD-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: 33283-11-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	8.026		Crippen Method
rinpol	2812.00		NIST Webbook
rinpol	2826.00		NIST Webbook
rinpol	2851.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C33283113&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

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