

Pregnan-17-ol, 3,20-bis[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»,20S)-

Other names:

5«beta»-Pregnan-17-ol, 3«alpha»,20«alpha»-bis(trimethylsiloxy)-

3«alpha»,20«alpha»-Bis-trimethylsilyl-ether of

5«beta»-pregnane-3«alpha»,17«alpha»,20«alpha»-triol

3,20-Bis[(trimethylsilyl)oxy]pregnan-17-ol-, (3«alpha»,5«beta»,20S)-

(3«alpha»,5«beta»)-3,20-Bis[(Trimethylsilyl)oxy]pregnan-17-ol

5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha»-triol, (3,20-O)-diTMSi

5«beta»-pregnane-3«alpha»,17«alpha»,20«beta»-triol, 3,20-bis-TMS

Pregnane-3,17,20-triol, (3«alpha»,5«beta»,20s)-, 2tms derivative

Inchi:

InChI=1S/C27H52O3Si2/c1-19(29-31(4,5)6)27(28)17-14-24-22-11-10-20-18-21(30-32(7,8)9)33

InchiKey:

PYOLIIABYCOZPT-UHFFFAOYSA-N

Formula:

C27H52O3Si2

SMILES:

CC(O[Si](C)(C)C)C1(O)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]:

480.87

CAS:

17562-94-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	7.220		Crippen Method
rinpol	2920.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2988.60		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C17562946&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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