

3,25-Bis[(trimethylsilyl)oxy]cholest-5-ene, (3«beta»)-

Other names:

Silane, [[(3«beta»)-cholest-5-ene-3,25-diy]bis(oxy)]bis(trimethyl-
Silane, (cholest-5-en-3«beta»,25-ylenedioxy)bis(trimethyl-
25-Hydroxycholesterol, (2TMS)
5-Cholesten-3«beta»,25-diol, diTMS
5-Cholesten-3beta,25-diol, bisTMS
Cholesterol, 25-hydroxy, bis-TMS
Cholesterol, 25-hydroxy, TMS
5-Cholesten-3B,25-diol, TMS
25-Hydroxycholesterol, di(trimethylsilyl) ether
5-Cholesten-3-«beta»,25-diol, TMS
25-Hydroxycholesterol, TMS
25-Hydroxycholesterol, 2tms derivative

Inchi:

InChI=1S/C33H62O2Si2/c1-24(13-12-20-31(2,3)35-37(9,10)11)28-16-17-29-27-15-14-25

InchiKey:

GIKJLUWETSCXLS-UHFFFAOYSA-N

Formula:

C33H62O2Si2

SMILES:

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

Mol. weight [g/mol]:

547.02

CAS:

33287-27-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	10.222		Crippen Method
rinqol	3399.00		NIST Webbook
rinqol	3405.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C33287273&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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