

Silane, trimethyl[[(3«beta»,5«alpha»)-stigmastan-3-yl]oxy]

Other names:

3-[(Trimethylsilyl)oxy]stigmastane, (3«beta»,5«alpha»)-

Stigmastanol, trimethylsilyl ether

5,6-Dihydro-«beta»-sitosterol, TMS

(24R)-24-Ethyl-5«alpha»-cholestan-3«beta»-ol, TMS

Stigmastane, 3-[(trimethylsilyl)oxy]-, (3«beta»,5«alpha»)-

Stigmastanol (24«beta»-ethyl-5«alpha»-cholestan-3«beta»-ol), TMS

(24R)-24-ethyl-5«alpha»-cholestan-3«beta»-ol (stigmastanol), TMS

Stigmastanol, tms derivative

Inchi: InChI=1S/C32H60OSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-3

InchiKey: TZWRPXXRQJDCPG-UHFFFAOYSA-N

Formula: C32H60OSi

SMILES: CCC(CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C(C)C

Mol. weight [g/mol]: 488.90

CAS: 55493-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	9.964		Crippen Method
rinpol	3348.00		NIST Webbook
rinpol	3349.00		NIST Webbook
rinpol	3343.00		NIST Webbook
rinpol	3349.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55493851&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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