

«beta»-Sitosterol trimethylsilyl ether

Other names:	Silane, trimethyl[[(3«beta»)-stigmast-5-en-3-yl]oxy]- Silane, trimethyl(stigmast-5-en-3«beta»-yloxy)- «beta»-Sitosterol TMS beta-Sitosterol, TMS 24«beta»-ethylcholest-5-en-3«beta»-ol, TMS Sitosterol (24«beta»-ethylcholest-5-en-3«beta»-ol), TMS Sitosterol, TMS «BETA»-sitosterol, tms derivative
Inchi:	InChI=1S/C32H58OSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-3
InchiKey:	XEWVATFZTBNDCE-OJDXYSFISA-N
Formula:	C32H58OSi
SMILES:	CCC(CCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	486.89
CAS:	2625-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	9.884		Crippen Method
rinpol	3344.00		NIST Webbook
rinpol	3348.00		NIST Webbook
rinpol	3296.00		NIST Webbook
rinpol	3356.00		NIST Webbook
rinpol	3344.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2625469&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/55-164-9/beta-Sitosterol-trimethylsilyl-ether.pdf>

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