Cholesterol trimethylsilyl ether

Other names:	Silane, [[(3«beta»)-cholest-5-en-3-yl]oxy]trimethyl-
	Silane, (cholesteryloxy)trimethyl-
	O-Trimethylsilylcholesterol
	3«beta»-(Trimethylsiloxy)cholest-5-ene
	Cholest-5-ene, 3-[(trimethylsilyl)oxy]-, (3«beta»)-
	Monotrimethylsilyl derivative of cholesterol
	3-[(Trimethylsilyl)oxy]cholest-5-ene-, 3.beta-
	5-Cholesten-3-«beta»-ol, TMS
	Cholesterol, TMS
	Cholesterol, mono-TMS
	Cholest-5-en-3«beta»-ol-, TMS
	5A-Cholesten-3-one, TMS
	Epicholesterol TMS
	Cholesterol (cholest-5-en-3«beta»-ol), TMS
	[[(3«beta»)-cholest-5-en-3-yl]oxy]trimethylsilane
	Cholesterol, tms derivative
Inchi:	InChI=1S/C30H54OSi/c1-21(2)10-9-11-22(3)26-14-15-27-25-13-12-23-20-24(31-32(6,7)8
InchiKey:	CBVJJGRSRFXUPK-SZXIZBHISA-N
Formula:	C30H54OSi
SMILES:	CC(C)CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	458.83
CAS:	1856-05-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.13		Crippen Method
logp	9.248		Crippen Method
rinpol	3101.00		NIST Webbook
rinpol	3135.00		NIST Webbook
rinpol	3144.90		NIST Webbook
rinpol	3120.00		NIST Webbook
rinpol	3122.00		NIST Webbook
rinpol	3143.00		NIST Webbook
rinpol	3155.00		NIST Webbook
rinpol	3132.00		NIST Webbook
rinpol	3110.00		NIST Webbook
rinpol	3144.90		NIST Webbook

rinpol	3124.00	NIST Webbook
rinpol	3136.00	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=C1856059&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices