3,16,17-Tris[(trimethylsilyl)oxy]estra-1,3,5(10)-trie
(16«beta»,17«beta»)-

Other names:	Silane, [(16«beta»,17«beta»)-estra-1,3,5(10)-triene-3,16,17-triyl]tris(oxy)]tris[trimethyl-
	Epiestriol, tris-(trimethylsilyl) ether
	16,17-Epiestriol, tri-TMS
	16,17-epi-Oestriol, tris-TMS
	16-epi-Oestriol, (3TMS)-
	16-epi-Oestriol, TMS
	16,17-Epiestriol, TMS
	16,17-epi-Oestriol, TMS
	16«BETA»,17«beta»-estriol, 3tms derivative
Inchi:	InChI=1S/C27H48O3Si3/c1-27-16-15-22-21-14-12-20(28-31(2,3)4)17-19(21)11-13-23(22
InchiKey:	MCKRDIGCTGOZEH-QWIJPDLKSA-N
Formula:	C27H48O3Si3
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]:	504.92
CAS:	57305-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	7.806		Crippen Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook
rinpol	2886.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2905.00		NIST Webbook
rinpol	2853.00		NIST Webbook
rinpol	2861.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305212&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