Silane, [[(16«beta»,17«alpha»)-estra-1,3,5(10)-triene-3,16,

Other names: Silane, [[(16«beta»,17«alpha»)-estra-1,3,5(10)-triene-3,16,17-triyl]tris(oxy)]tris*trimethyl-
3,16«beta»,17«alpha»-Trihydroxy-1,3,5(10)-estratriene 3,16,17-tms
16-Epiestriol, 3,16,17-tris(trimethylsilyl) ether
16«BETA»,17«alpha»-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-WTYWGGPZSA-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: 57305-22-3

Physical Properties

Property code	Value	Unit	Source
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-6.66		Cheméo Relay (1.0)
logp	7.806		Crippen Method
rinpol	2929.60		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2899.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tf	369.99	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305223&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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