Silane, (estra-1,3,5(10)-trien-3-yloxy)trimethyl-

Other names:	3-[(Trimethylsilyl)oxy]estra-1,3,5(10)-triene
	«beta»-Estradiol, TMS
	17-Deoxoestrone, tms derivative
Inchi:	InChI=1S/C21H32OSi/c1-21-12-5-6-20(21)19-9-7-15-14-16(22-23(2,3)4)8-10-17(15)18(1
InchiKey:	FXRPWGRCNHJNJG-UHFFFAOYSA-N
Formula:	C21H32OSi
SMILES:	CC12CCCC1C1CCc3cc(O[Si](C)(C)C)ccc3C1CC2
Mol. weight [g/mol]:	328.56
CAS:	29755-24-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	6.146		Crippen Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		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=C29755246&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/12-819-9/Silane-estra-1-3-5-10-trien-3-yloxy-trimethyl.pdf

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