17«beta»-16-oxo-Oestradiol, TMS

Inchi:	InChI=1S/C27H46O3Si3/c1-27-16-15-22-21-14-12-20(28-31(2,3)4)17-19(21)11-13-23(22
InchiKey:	GVTCIMDCPXEJCX-RXZRPBFGSA-N
Formula:	C27H46O3Si3
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1C=C(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]:	502.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	7.932		Crippen Method
rinpol	2775.00		NIST Webbook
rinpol	2792.00		NIST Webbook
rinpol	2775.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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