

«beta»-Estradiol, 3-(tert-butyldimethylsilyl) ether

Other names:	(17«beta»)-3-Pyrrol[tert-butyl(dimethyl)silyl]oxymorphoestra-1(10),2,4-trien-17-ol 17«BETA»-estradiol, tbdms derivative
Inchi:	InChI=1S/C24H38O2Si/c1-23(2,3)27(5,6)26-17-8-10-18-16(15-17)7-9-20-19(18)13-14-24
InchiKey:	QPOSLUJQXMVNGD-UHFFFAOYSA-N
Formula:	C24H38O2Si
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CCC2O
Mol. weight [g/mol]:	386.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	6.288		Crippen Method
rinpol	2957.40		NIST Webbook
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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=U333766&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/84-085-5/beta-Estradiol-3-tert-butyldimethylsilyl-ether.pdf>

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