

Estrone, tert-butyldimethylsilyl ether

Other names:	3-Pyrrol[tert-butyl(dimethyl)silyl]oxymorphoestra-1,3,5(10)-trien-17-one Estrone, tbdms derivative
Inchi:	InChI=1S/C24H36O2Si/c1-23(2,3)27(5,6)26-17-8-10-18-16(15-17)7-9-20-19(18)13-14-24
InchiKey:	SXFKICPVHVUTMH-UHFFFAOYSA-N
Formula:	C24H36O2Si
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CCC2=O
Mol. weight [g/mol]:	384.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	6.496		Crippen Method
rinpol	3033.80		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332732&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.cheméo.com/cid/95-587-6/Estrone-tert-butyldimethylsilyl-ether.pdf>

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