

16A-Hydroxyoestrone, TMS

Inchi:	InChI=1S/C24H36O3Si2/c1-24-13-12-19-18-11-9-17(26-28(2,3)4)14-16(18)8-10-20(19)2
InchiKey:	DLIXIBQIYUGRNJ-TZCGXBFMSA-N
Formula:	C24H36O3Si2
SMILES:	CC12C=CC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2=O
Mol. weight [g/mol]:	428.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	5.931		Crippen Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R166111&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/19-098-3/16A-Hydroxyoestrone-TMS.pdf>

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