

# Estra-1,3,5(10)-trien-17-one, 3,16«alpha»-bis(trimethylsiloxy)-

Other names:	16«alpha»-Hydroxyestrone, TMS
Inchi:	InChI=1S/C24H38O3Si2/c1-24-13-12-19-18-11-9-17(26-28(2,3)4)14-16(18)8-10-20(19)2
InchiKey:	OTOYHXDNWUYSAL-QMDPOKHVSA-N
Formula:	C24H38O3Si2
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2=O
Mol. weight [g/mol]:	430.73
CAS:	28416-72-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	6.155		Crippen Method
rinpola	2748.00		NIST Webbook
rinpola	2762.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C28416720&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28416720&amp;Units=SI</a>

## Legend

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

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