

# 5«alpha»-Estranediol-3«beta»,17«beta», bis-TMS

Other names:	5A-Estran-3B,17B-diol, bis-TMS
Inchi:	InChI=1S/C24H46O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey:	UOQHQB NVJDUSEX-NKWIKOKZSA-N
Formula:	C24H46O2Si2
SMILES:	CC12CCC3C4CCC(O[Si](C)(C)C)CC4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]:	422.79

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	7.079		Crippen Method
rmpol	2540.00		NIST Webbook
rmpol	2558.00		NIST Webbook
rmpol	2573.00		NIST Webbook
rmpol	2540.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R92296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R92296&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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