

5«alpha»-Estranediol-3«alpha»,17«beta»,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:	UOQHQBUNVJDUSEX-DMGKZOFXSA-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
rinpol	2491.00		NIST Webbook
rinpol	2502.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R297700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/54-564-6/5-alpha-Estranediol-3-alpha-17-beta-bis-TMS.pdf>

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