

«beta»-Testosterone, TMS

Other names:	Testosterone, bis-TMS (2,4-diene) Androst-4-en-3-on-17B-ol, TMS
Inchi:	InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	OGAHQMPXQGCDNO-MCZOVZSXSA-N
Formula:	C25H44O2Si2
SMILES:	CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	7.515		Crippen Method
rinpola	2630.00		NIST Webbook
rinpola	2606.00		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=R81976&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-914-2/beta-Testosterone-TMS.pdf>

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