

4-Chlorodehydromethyltestosterone, per-TMS

Other names:	4-Chloro-1,2-dehydro-17«alpha»-methyltestosterone, bis-TMS
Inchi:	InChI=1S/C26H43ClO2Si2/c1-24-15-14-22(28-30(4,5)6)23(27)21(24)11-10-18-19(24)12-
InchiKey:	GBKVYVYEVCCEMU-UHFFFAOYSA-N
Formula:	C26H43ClO2Si2
SMILES:	CC12C=CC(O[Si](C)(C)C)=C(Cl)C1=CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	479.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	8.247		Crippen Method
rinpol	2931.00		NIST Webbook
rinpol	2993.00		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=R258067&Units=SI

Legend

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

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<https://www.chemeo.com/cid/52-974-3/4-Chlorodehydromethyltestosterone-per-TMS.pdf>

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