

17-epi-4-Chlorodehydromethyltestosterone, 17-TMS

Inchi:	InChI=1S/C23H35ClO2Si/c1-21-12-11-19(25)20(24)18(21)8-7-15-16(21)9-13-22(2)17(15)
InchiKey:	QMMLRALJVSNRHB-BLAZJUBZSA-N
Formula:	C23H35ClO2Si
SMILES:	CC12C=CC(=O)C(Cl)=C1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	407.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	6.471		Crippen Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R257633&Units=SI

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/27-575-4/17-epi-4-Chlorodehydromethyltestosterone-17-TMS.pdf>

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