

4-Chloro-17A-methyl-1,4-abdrosten-3-one-6B,17B

di-TMS

Other names:	6«beta»-Hydroxy-4-Chloro-1,2,dehydro-17«alpha»-methyltestosterone, bis-TMS
Inchi:	InChI=1S/C26H43ClO3Si2/c1-24-13-12-20(28)23(27)22(24)21(29-31(4,5)6)16-17-18(24)
InchiKey:	TYFGLBZGTXUKIU-QVKCDFLLSA-N
Formula:	C26H43ClO3Si2
SMILES:	CC12C=CC(=O)C(Cl)=C1C(O[Si](C)(C)C)CC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	495.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	7.301		Crippen Method
rinpol	3001.00		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=R61522&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/19-927-2/4-Chloro-17A-methyl-1-4-abdrosten-3-one-6B-17B-diol-di-TMS.pdf>

Generated by Cheméo on 2024-04-27 19:38:05.504448623 +0000 UTC m=+16535934.425025933.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.