

Androst-4-en-4-chloro-3«alpha»-ol-17-one, TMS

Inchi:	InChI=1S/C25H43ClO2Si2/c1-24-16-14-21(27-29(3,4)5)23(26)20(24)10-9-17-18-11-12-2
InchiKey:	SHTZVTGOIGPHTA-CJJLFJDWSA-N
Formula:	C25H43ClO2Si2
SMILES:	CC12CCC3C(CCC4=C(CI)C(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]:	467.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.081		Crippen Method
rinpol	2720.00		NIST Webbook
rinpol	2736.00		NIST Webbook
rinpol	2720.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/39-843-3/Androst-4-en-4-chloro-3-alpha-ol-17-one-TMS.pdf>

Generated by Cheméo on 2024-04-29 23:11:32.164698589 +0000 UTC m=+16721541.085275900.

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