

Androst-1,4-dien-17«alpha»-methyl-4-chloro-17«b

TMS

InChI=1S/C26H43ClO2Si2/c1-24-15-14-22(28-30(4,5)6)23(27)21(24)11-10-18-19(24)12-

GBKVYVYEVCEEMU-KEGRRINUSA-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	2977.00		NIST Webbook
rinpol	2990.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R322004&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/12-589-5/Androst-1-4-dien-17-alpha-methyl-4-chloro-17-beta-ol-3-one-TMS.pdf>

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