

Dehydrochlorotestosterone (Androst-1,4-dien-17A-methyl-4-chloro-17B-ol-3-ol-TMS)

TMS
InchiKey:

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

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
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Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U412282&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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