

Epitestosterone (Androst-4-en-17A-ol-3-one), TMS

Inchi: InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-28)25
InchiKey: OGAHQMPXQGCNO-RRLSKXGXSA-N
Formula: C₂₅H₄₄O₂Si₂
SMILES: CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	7.515		Crippen Method
rinpol	2645.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585567&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/23-776-5/Epitestosterone-Androst-4-en-17A-ol-3-one-TMS.pdf>

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