

trans-Dehydroandrosterone, tert-butyl dimethylsilyl ether

Other names:

(3«beta»)-3-Pyrrol[tert-butyl(dimethyl)silyl]oxymorphoandrost-5-en-17-one
Dehydroepiandrosterone, (e)-, tbdms derivative

Inchi: InChI=1S/C25H42O2Si/c1-23(2,3)28(6,7)27-18-12-14-24(4)17(16-18)8-9-19-20-10-11-22

InchiKey: BGIQEPPPFKLP-UHFFFAOYSA-N

Formula: C₂₅H₄₂O₂Si

SMILES: CC12CCC3C(CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 402.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	6.909		Crippen Method
rinpol	2892.30		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=U333789&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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