

11B-Hydroxyandrosterone (5A-Androstan-3A,11B-diol-17-one), TMS

Inchi: InChI=1S/C25H46O3Si2/c1-24-14-13-18(27-29(3,4)5)15-17(24)9-10-19-20-11-12-22(26)
InchiKey: SVZGBEADGIZYEM-CQAIBLENSA-N
Formula: C25H46O3Si2
SMILES: CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 450.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	6.648		Crippen Method
rinpol	2696.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585354&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/32-154-5/11B-Hydroxyandrosterone-5A-Androstan-3A-11B-diol-17-one-TMS.pdf>

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