

Androst-5-en-3«beta»,17«alpha»-diol, TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: YXSPGYZGGCSNLG-YRQMLZPGSA-N
Formula: C25H46O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	7.389		Crippen Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R321952&Units=SI>

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/56-127-9/Androst-5-en-3-beta-17-alpha-diol-TMS.pdf>

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