

5«beta»-Androst-1-ene-3«beta»,17«alpha»-diol, per-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(27-28)/h1-24,26-28H,25H2,29H4
InChIKey: AFIXZMQBNBXTRZ-ZQJZVJABSA-N

Formula: C₂₅H₄₆O₂Si₂

SMILES: CC12C=CC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	7.245		Crippen Method
rinpol	2464.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2464.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R518473&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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<https://www.cheméo.com/cid/17-645-7/5-beta-Androst-1-ene-3-beta-17-alpha-diol-per-TMS.pdf>

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