

# 5«alpha»-Androst-1-ene-3«alpha»,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)25/s1-24,15-13,19,26-28,3,4,5,17-18,24,9-10,20-21,11-12,23,27-28,25/h1-24,15-13,19,26-28,3,4,5,17-18,24,9-10,20-21,11-12,23,27-28,25/t1-24,15-13,19,26-28,3,4,5,17-18,24,9-10,20-21,11-12,23,27-28,25

InChIKey: AFIXZMQBNBXTRZ-CKFIOJRASA-N

Formula: C<sub>25</sub>H<sub>46</sub>O<sub>2</sub>Si<sub>2</sub>

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	2474.00		NIST Webbook
rinpol	2523.00		NIST Webbook
rinpol	2474.00		NIST Webbook

## Sources

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R518413&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

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