

5«alpha»-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-NGAZGVGCSA-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	2554.00		NIST Webbook
rinpol	2619.00		NIST Webbook
rinpol	2554.00		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=R518433&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.cheméo.com/cid/63-250-4/5-alpha-Androst-1-ene-3-beta-17-alpha-diol-per-TMS.pdf>

Generated by Cheméo on 2025-12-05 18:25:34.246045544 +0000 UTC m=+4707331.776086199.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.