

Androst-4-en-3,17-dione, TMS

Inchi: InChI=1S/C25H42O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: QFNPJAZQCOZTRB-SWSPXDAHSA-N
Formula: C25H42O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)=CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12
Mol. weight [g/mol]: 430.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	7.640		Crippen Method
rinpol	2678.00		NIST Webbook
rinpol	2684.00		NIST Webbook
rinpol	2678.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R321927&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/33-746-7/Androst-4-en-3-17-dione-TMS.pdf>

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