

5B-Androstan-3-on-17B-ol, 17A-methyl, TMS

Inchi: InChI=1S/C26H48O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InchiKey: STULRMPZBKMPMD-VDVKYTFTSA-N
Formula: C₂₆H₄₈O₂Si₂
SMILES: CC12CC=C(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 448.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	7.985		Crippen Method
rinpol	2605.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92353&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.chemeo.com/cid/56-568-0/5B-Androstan-3-on-17B-ol-17A-methyl-TMS.pdf>

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