

17-«alpha»-Methyl-5-«beta»-androstan-3-«alpha», per-TMS

Other names:

5B-androstan-3A,17B-diol, 17A-methyl, bis-TMS

17A-Methyl-5B-androstan-3A,17B-diol, di-TMS

Inchi: InChI=1S/C26H50O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25

InchiKey: GNQZRHQPXWSWJC-YDGBGVRZSA-N

Formula: C26H50O2Si2

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]: 450.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.859		Crippen Method
rinpol	2620.00		NIST Webbook
rinpol	2637.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R61451&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/49-476-0/17-alpha-Methyl-5-beta-androstan-3-alpha-17-beta-diol-per-TMS.pdf>

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