

5«alpha»-Androstan-17«alpha»-methyl-3',17«beta»

TMS

InChI=1S/C27H48N2O2Si2/c1-25-17-20-23(28-29-24(20)30-32(4,5)6)16-18(25)10-11-19

InchiKey:

VWZNMOCSGFOJFR-WHAJAHTISA-N

Formula:

C27H48N2O2Si2

SMILES:

CC12Cc3c(n[nH]c3O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]:

488.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	6.709		Crippen Method
rinpol	3221.00		NIST Webbook
rinpol	3207.00		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=R321987&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.chemeo.com/cid/21-592-1/5-alpha-Androstan-17-alpha-methyl-3-17-beta-diol-3-2c-pyrazol-TMS.pdf>

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