

5«alpha»-Androstan-17«alpha»-methyl-4«beta»,17

TMS

InchiKey:

InChI=1S/C27H48N2O2Si2/c1-25-16-18-17-28-29-23(18)24(30-32(4,5)6)22(25)11-10-19

AZJYUUNJZKMMLR-YZNVKJLLSA-N

Formula:

C27H48N2O2Si2

SMILES:

CC12Cc3c[nH]nc3C(O[Si](C)(C)C)C1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]:

488.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	6.845		Crippen Method
rinpol	3233.00		NIST Webbook
rinpol	3216.00		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=R321992&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/34-631-3/5-alpha-Androstan-17-alpha-methyl-4-beta-17-beta-diol-3-2c-pyrazol-TMS.pdf>

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