

5«beta»-Androstan-7«alpha»,17«alpha»-dimethyl-

TMS

InchiKey:

InChI=1S/C27H52O2Si2/c1-19-17-20-18-21(28-30(5,6)7)11-14-25(20,2)22-12-15-26(3)2

TWYZBBIZYQXGMM-MVCACVFXSA-N

Formula:

C27H52O2Si2

SMILES:

CC1CC2CC(O[Si](C)(C)C)CCC2(C)C2CCC3(C)C(CCC3(C)O[Si](C)(C)C)C12

Mol. weight [g/mol]:

464.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		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=R321898&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/52-880-7/5-beta-Androstan-7-alpha-17-alpha-dimethyl-3-alpha-17-beta-diol-TMS.pdf>

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