

5-«alpha»-Androst-1-ene-3-«beta»,17-«beta»-diol,

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

AFIXZMQBNBXTRZ-MWZFTKEVSA-N

C25H46O2Si2

CC12C=CC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	7.245		Crippen Method
rinpol	2652.00		NIST Webbook
rinpol	2642.00		NIST Webbook
rinpol	2603.00		NIST Webbook
rinpol	2678.00		NIST Webbook
rinpol	2652.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R384700&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/10-423-0/5-alpha-Androst-1-ene-3-beta-17-beta-diol-TMS.pdf>

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