

3«alpha»,17«beta»-Dihydroxy-5«alpha»-androstane

TMS

InchiKey:

InChI=1S/C25H46O3Si2/c1-24-13-11-17(27-29(3,4)5)15-21(24)22(26)16-18-19-9-10-23(

YGPPARABFBKEMI-XAEDEZGWSA-N

Formula:

C25H46O3Si2

SMILES:

CC12CCC3C(CC(=O)C4CC(O[Si](C)(C)C)CCC43C)C1CCC2O[Si](C)(C)C

Mol. weight [g/mol]:

450.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	6.648		Crippen Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		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=R306948&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/27-460-1/3-alpha-17-beta-Dihydroxy-5-alpha-androstan-6-one-TMS.pdf>

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