

3«alpha»,16«alpha»-dihydroxy-5«beta»-androstane

TMS

InchiKey:

InChI=1S/C25H46O3Si2/c1-24-13-11-18(27-29(3,4)5)15-17(24)9-10-19-20(24)12-14-25(

JTMVSMYLSJYTE-KAVSHOJGSA-N

Formula:

C₂₅H₄₆O₃Si₂

SMILES:

CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC(O[Si](C)(C)C)C2=O

Mol. weight [g/mol]:

450.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	6.648		Crippen Method
rinpol	2604.00		NIST Webbook
rinpol	2556.00		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=R488189&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/68-784-7/3-alpha-16-alpha-dihydroxy-5-beta-androstan-17-one-TMS.pdf>

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