

3«beta»,16«alpha»-dihydroxy-5-androsten-17-one

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H44O3Si2/c1-24-13-11-18(27-29(3,4)5)15-17(24)9-10-19-20(24)12-14-25(

BDPGVCUMZYXUEQ-QEBUGNDYSA-N

C25H44O3Si2

CC12CCC3C(CC=C4CC(O[Si](C)(C)C)CCC43C)C1CC(O[Si](C)(C)C)C2=O

448.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	6.568		Crippen Method
rinpol	2699.00		NIST Webbook
rinpol	2668.00		NIST Webbook
rinpol	2699.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R488218&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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