

3«beta»-Hydroxy-5«alpha»-androstane-6,17-dione

TMS

InchiKey:

InChI=1S/C25H44O3Si2/c1-24-13-11-17(27-29(3,4)5)15-21(24)22(26)16-18-19-9-10-23(

ROUPNNKSTWCYDL-GMPWYMRSSA-N

Formula:

C₂₅H₄₄O₃Si₂

SMILES:

CC12CCC3C(CC(=O)C4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C

Mol. weight [g/mol]:

448.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	6.774		Crippen Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R307010&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/38-775-0/3-beta-Hydroxy-5-alpha-androstane-6-17-dione-TMS.pdf>

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