

3-«beta»-Hydroxy-5-androsten-11,17-dione, TMS

Inchi:	InChI=1S/C23H37NO3Si/c1-22-12-11-16(27-28(4,5)6)13-15(22)7-8-17-18-9-10-20(24-26)
InchiKey:	NHDNWLWKVCPZBJ-HDSYMABGSA-N
Formula:	C23H37NO3Si
SMILES:	CON=C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3C(=O)CC12C
Mol. weight [g/mol]:	403.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	5.351		Crippen Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		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=R386068&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/53-280-2/3-beta-Hydroxy-5-androsten-11-17-dione-TMS.pdf>

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