

3-«beta»,19-Dihydroxy-5-androsten-17-one, TMS

Inchi:	InChI=1S/C25H44O3Si2/c1-24-14-12-19(28-30(5,6)7)16-18(24)8-9-20-21(24)13-15-25(1
InchiKey:	VQMMMQOJOBSNGT-SSBCDWDPSA-N
Formula:	C25H44O3Si2
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(CO[Si](C)(C)C)C(=O)CCC12
Mol. weight [g/mol]:	448.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	6.570		Crippen Method
rinpol	2685.00		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=R386048&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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