

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

Other names:	17«BETA»-hydroxy-5«alpha»-androstane-3,6-dione, tms derivative
Inchi:	InChI=1S/C22H36O3Si/c1-21-10-8-14(23)12-18(21)19(24)13-15-16-6-7-20(25-26(3,4)5)2
InchiKey:	DPRDHSNOPIJZCX-JEJUZZDKSA-N
Formula:	C22H36O3Si
SMILES:	CC12CCC3C(CC(=O)C4CC(=O)CCC43C)C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]:	376.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	4.997		Crippen Method
rinsol	2920.00		NIST Webbook
rinsol	2920.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U69382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/84-534-6/17-beta-Hydroxy-5-alpha-androstane-3-6-dione-TMS.pdf>

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