

5«beta»-Androst-1-ene-3«beta»,17«beta»-diol,bis-

Other names:	5«beta»-Androst-1-ene-3«beta»,17«beta»-diol, per-TMS
Inchi:	InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	AFIXZMQBNBXTRZ-TZJCIHJTSA-N
Formula:	C25H46O2Si2
SMILES:	CC12C=CC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	7.245		Crippen Method
rinpol	2541.00		NIST Webbook
rinpol	2608.00		NIST Webbook
rinpol	2571.00		NIST Webbook
rinpol	2575.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R319345&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
rinpol:	Non-polar retention indices

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<https://www.cheméo.com/cid/69-668-5/5-beta-Androst-1-ene-3-beta-17-beta-diol-bis-TMS.pdf>

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