

17a-Methyl-5a-androstan-3a,17b-diol ditms

Other names:	17-«alpha»-Methyl-5-«alpha»-androstan-3-«alpha»,17-«beta»-diol, per-TMS 5A-Androstan-3A,17B-diol, 17A-methyl, bis-TMS 17«ALPHA»-methyl-5«alpha»-androstane-3«alpha»,17«beta»-diol, 2tms derivative
Inchi:	InChI=1S/C26H50O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InchiKey:	GNQZRHQPXWSWJC-UHFFFAOYSA-N
Formula:	C26H50O2Si2
SMILES:	CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	450.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.859		Crippen Method
rinpol	2615.00		NIST Webbook
rinpol	2634.00		NIST Webbook

Sources

Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U331737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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