17«alpha»-Methyl-6«beta»,17«beta»-dihydroxy-1,4 bis(trimethylsilyl)

Other names:	17-Methyl-6,17-bis[(trimethylsilyl)oxy]androsta-1,4-dien-3-one, (6«beta»,17«beta»)- 6-«beta»-Hydroxymetandienone, per-TMS 6«beta»-Hydroxy-Methandienone, bis-TMS 6«BETA»-hydroxymethandienone, 2tms derivative
Inchi:	InChI=1S/C26H44O3Si2/c1-24-13-10-18(27)16-22(24)23(28-30(4,5)6)17-19-20(24)11-14
InchiKey:	RAKGZQRFODNUHY-UHFFFAOYSA-N
Formula:	C26H44O3Si2
SMILES:	CC12C=CC(=O)C=C1C(O[Si](C)(C)C)CC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	460.80
CAS:	67896-65-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	6.735		Crippen Method
rinpol	2919.00		NIST Webbook
rinpol	2915.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67896655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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