17-«alpha»-Hydroxy-17-«beta»-methyl-5-«beta»-an per-TMS

Inchi:	InChI=1S/C26H48O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InchiKey:	QMJUKIBVQVZILS-JESIWLCVSA-N
Formula:	C26H48O2Si2
SMILES:	CC12CCC(O[Si](C)(C)C)=CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]:	448.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	7.985		Crippen Method
rinpol	2498.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R257168&Units=SI

Legend

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

Latest version available from:
https://www.chemeo.com/cid/52-316-3/17-alpha-Hydroxy-17-beta-methyl-5-beta-androstan-3-one-per-TMS.pdf
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