17-«alpha»-Methyl-5-«beta»-androst-1-ene-3-«alpha»-17-«beta»-diol-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(2)23(21)14-17-26(25,3)28-30(7,8)9/h10,20-23H,11-17H2,1-9H3/t20-,21-,22-,23-,24+,25+,26+/m1/s1

InchiKey: FKXKDLQNCNDLSD-YDGBGVRZSA-N

Formula: C26H48O2Si2

SMILES: CC12C=CC(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	-3.19		Crippen Method
logp	7.635		Crippen Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R257282&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices