17A-(2-Methoxy)oestradiol, TMS

Inchi: InChI=1S/C25H42O3Si2/c1-25-14-13-18-19(21(25)11-12-24(25)28-30(6,7)8)10-9-17-15-
InchiKey: FLTQSMBAZOOLHF-OFGFBFBPSA-N
Formula: C25H42O3Si2
SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 446.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	6.985		Crippen Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R166260&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