6-Dehydroestradiol, TMS

Inchi: InChI=1S/C24H38O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey: TZVQVTRWZGEMHS-WQABULOPSA-N
Formula: C24H38O2Si2
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4C=CC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 414.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	7.057		Crippen Method
rinpol	2657.00		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=R166413&Units=SI

Legend

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