1,3,5(10)-Oestratrien-17«alpha»-ol, TMS

Inchi: InChI=1S/C21H32OSi/c1-21-14-13-17-16-8-6-5-7-15(16)9-10-18(17)19(21)11-12-20(21)2
InchiKey: WIQSXNCXAZKRKG-JRSUCEMESA-N
Formula: C21H32OSi
SMILES: CC12CCC3c4ccccc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 328.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	5.763		Crippen Method
rinpol	2238.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2238.00		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=R523707&Units=SI

Legend

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