1,3,5(10)-Oestratriene-2,3,17«beta»-triol, 2,3-TMS-17-HFB

Inchi: InChI=1S/C28H39F7O4Si2/c1-25-13-12-17-18(20(25)10-11-23(25)37-24(36)26(29,30)27

InchiKey: SGXGBWWIMINUGQ-WYKNMPDOSA-N

Formula: C28H39F7O4Si2

SMILES: CC12CCC3c4cc(O[Si](C)(C)C)c(O[Si](C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C

Mol. weight [g/mol]: 628.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	8.715		Crippen Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		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=R537127&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices