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

Inchi: InChI=1S/C26H33F7O4Si/c1-23-11-10-15-16(7-6-14-12-20(37-38(3,4)5)19(35-2)13-17(1

InchiKey: IYAZYUBXQIGZGF-IGRNSJNGSA-N

Formula: C26H33F7O4Si

SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC12

Mol. weight [g/mol]: 570.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	7.510		Crippen Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		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=R537192&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices