1,3,5(10)-Oestratriene-3,17«alpha»-diol, 3-TMS-17-HFB

Inchi: InChI=1S/C25H31F7O3Si/c1-22-12-11-17-16-8-6-15(35-36(2,3)4)13-14(16)5-7-18(17)19

InchiKey: SKCZEAZINGMGHC-SXFAUFNYSA-N

Formula: C25H31F7O3Si

SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 540.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	7.501		Crippen Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537216&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