1,3,5(10)-Oestratriene-2-methoxy-3,16«alpha»,17« 3-TBDMS-16,17-TFA

Inchi: InChI=1S/C29H38F6O6Si/c1-26(2,3)42(6,7)41-21-12-15-8-9-17-16(18(15)13-20(21)38-5)

InchiKey: ROZNEEBOYMMKNK-HCVCXDRWSA-N

Formula: C29H38F6O6Si

SMILES: COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)F)C2OC(=O

Mol. weight [g/mol]: 624.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	7.493		Crippen Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		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=R537167&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices