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

Inchi:	InChI=1S/C33H38F14O6Si/c1-26(2,3)54(6,7)53-21-12-15-8-9-17-16(18(15)13-20(21)50-
InchiKey:	UOSOILWREVGMGP-HCVCXDRWSA-N
Formula:	C33H38F14O6Si
SMILES:	COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)C(F)
Mol. weight [g/mol]:	824.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.61		Crippen Method
logp	10.035		Crippen Method
rinpol	2864.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537147&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

Latest version available from:
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