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

Inchi: InChI=1S/C31H38F10O6Si/c1-26(2,3)48(6,7)47-21-12-15-8-9-17-16(18(15)13-20(21)44-
InchiKey: GGYUTFKHRNZRGB-HCVCXDRWSA-N
Formula: C31H38F10O6Si
SMILES: COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)F)C2
Mol. weight [g/mol]: 724.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.15		Crippen Method
logp	8.764		Crippen Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537152&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

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