1,3,5(10)-Oestratriene-3,17«beta»-diol, 3-TBDMS-17-HFB

Inchi: InChI=1S/C28H37F7O3Si/c1-24(2,3)39(5,6)38-17-8-10-18-16(15-17)7-9-20-19(18)13-14-

InchiKey: VXSFHPHMTCEVAL-LCIIEAPSSA-N

Formula: C28H37F7O3Si

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

Mol. weight [g/mol]: 582.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.55		Crippen Method
logp	8.671		Crippen Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537236&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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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