6«beta»-Hydroxy-Fluoxymesterone, tetra-TMS (3,5-diene)

Inchi: InChI=1S/C32H61FO4Si4/c1-29-18-16-23(34-38(4,5)6)20-26(29)27(35-39(7,8)9)21-25-2

InchiKey: PDSJFWRYSJSVQU-MCLMALPUSA-N

Formula: C32H61FO4Si4

SMILES: CC1(O[Si](C)(C)C)CCC2C3CC(O[Si](C)(C)C)=C4C=C(O[Si](C)(C)C)CCC4(C)C3(F)C(O[

Mol. weight [g/mol]: 641.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	10.006		Crippen Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R263113&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:

https://www.chemeo.com/cid/52-315-4/6-beta-Hydroxy-Fluoxymesterone-tetra-TMS-3-5-diene.pdf

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