Fluoxymesterone, tris-TMS (3,5-diene)

Other names:	Fluoxymesterone, tri-TMS
Inchi:	InChI=1S/C29H53FO3Si3/c1-26-17-15-22(31-34(4,5)6)19-21(26)13-14-24-23-16-18-28(3
InchiKey:	WDLOCDDPAONUQC-CDNMOJTGSA-N
Formula:	C29H53FO3Si3
SMILES:	CC1(O[Si](C)(C)C)CCC2C3CC=C4C=C(O[Si](C)(C)C)CCC4(C)C3(F)C(O[Si](C)(C)C)CC
Mol. weight [g/mol]:	552.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	8.827		Crippen Method
rinpol	2935.00		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=R61657&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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