

Fluoxymesterone, tris-TMS (2,4-diene)

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: RWIFRBGFXNTZQI-GLBXAPIRSA-N
Formula: C29H53FO3Si3
SMILES: CC1(O[Si](C)(C)C)CCC2C3CCC4=CC(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	2890.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263188&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/69-568-6/Fluoxymesterone-tris-TMS-2-4-diene.pdf>

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