

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

Inchi: InChI=1S/C26H45FO3Si2/c1-23-14-12-19(29-31(4,5)6)16-18(23)10-11-21-20-13-15-25(3)
InchiKey: QMJFBQBJKSMDMS-TWFUYWQQSA-N
Formula: C26H45FO3Si2
SMILES: CC1(O)CCC2C3CC=C4C=C(O[Si](C)(C)C)CCC4(C)C3(F)C(O[Si](C)(C)C)CC21C
Mol. weight [g/mol]: 480.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	6.968		Crippen Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263168&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/32-985-3/Fluoxymesterone-bis-TMS-3-5-diene.pdf>

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