Androst-4-en-9«alpha»-fluoro-17«alpha»-methyl-3 TMS

InChI: InChI=1S/C32H63FO4Si4/c1-29-18-16-23(34-38(4,5)6)20-26(29)27(35-39(7,8)9)21-25-2

InchiKey: UUYYWGFQQAOGRS-UHFFFAOYSA-N

Formula: C32H63FO4Si4

SMILES: CC1(O[Si](C)(C)C)CCC2C3CC(O[Si](C)(C)C)C4=CC(O[Si](C)(C)C)CCC4(C)C3(F)C(O[S

Mol. weight [g/mol]: 643.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.65		Crippen Method
logp	9.532		Crippen Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U412255&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