Formebelone M (Androst-1,4-dien-2z-hydroxymethyl-17A-methyl-1 TMS

Inchi: InChI=1S/C33H62O4Si4/c1-31-21-24(23-34-38(4,5)6)28(35-39(7,8)9)20-25(31)16-17-26-

InchiKey: BDCWZCKSOOQPMQ-UHFFFAOYSA-N

Formula: C33H62O4Si4

SMILES: CC12C=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)=CC1=CCC1C2C(O[Si](C)(C)C)CC2(C)C1CC

Mol. weight [g/mol]: 635.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	9.732		Crippen Method
rinpol	3096.00		NIST Webbook
rinpol	3096.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U412257&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