6«alpha»-Methylprednisolone, tetra-TMS

Inchi: InChI=1S/C34H62O5Si4/c1-24-20-26-27-17-19-34(39-43(13,14)15,30(35)23-36-40(4,5)6
InchiKey: FEUBEJZGKUBSGR-JVJUJFTESA-N
Formula: C34H62O5Si4
SMILES: CC1=C2C=C(O[Si](C)(C)C)C=CC2(C)C2C(O[Si](C)(C)C)CC3(C)C(CCC3(O[Si](C)(C)C)C
Mol. weight [g/mol]: 663.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	9.301		Crippen Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R557903&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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