16«alpha»-Methylpregnenolone, TMS

Inchi: InChI=1S/C25H42O2Si/c1-16-14-22-20-9-8-18-15-19(27-28(5,6)7)10-12-24(18,3)21(20)1

InchiKey: JOYGRUHLOYRWGM-BXWWMJJPSA-N

Formula: C25H42O2Si

SMILES: CC(=O)C1C(C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 402.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	6.621		Crippen Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305143&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices