5-Pregnen-3-«beta»-ol-11-one, MO-TMS

Inchi: InChI=1S/C25H43NO2Si/c1-8-17-10-12-21-20-11-9-18-15-19(28-29(5,6)7)13-14-24(18,2
InchiKey: MRYWMVXCCWMGNO-WYTYWXAZSA-N
Formula: C25H43NO2Si
SMILES: CCC1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]: 417.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	6.808		Crippen Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R487220&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