4-Pregnen-3-«beta»,11-«beta»-diol, TMS

Inchi: InChI=1S/C27H50O2Si2/c1-10-19-12-14-23-22-13-11-20-17-21(28-30(4,5)6)15-16-26(20
InchiKey: KWOODOOLPJTRQL-RMGMAWNNSA-N
Formula: C27H50O2Si2
SMILES: CCC1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 462.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	8.026		Crippen Method
rinpol	2692.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486267&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