5-«alpha»-Pregnan-20-«beta»-ol-11-one, MO-TMS

Inchi: InChI=1S/C25H45NO2Si/c1-17(28-29(5,6)7)20-13-14-21-19-12-11-18-10-8-9-15-24(18,2

InchiKey: AENBXJWUEFXGGT-TWRCBNSESA-N

Formula: C25H45NO2Si

SMILES: CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CCCCC3(C)C12

Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2660.00		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=R486470&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices