*5«beta»-Pregnane-3«alpha», 20«beta»-diol-11-one, MO TMS

Inchi: InChI=1S/C26H49NO3Si2/c1-17(29-31(3,4)5)20-13-14-22-23-11-9-18-15-19(30-32(6,7)8
InchiKey: MOUGWOFPPKPNTL-WIKYTUNOSA-N
Formula: C26H49NO3Si2
SMILES: CON=C1CC2C(C(C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3C12
Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	6.938		Crippen Method
rinpol	2886.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250281&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