4-Pregnen-3-«beta»,11-«beta»-diol-20-one, MO-TMS

Inchi: InChI=1S/C28H51NO3Si2/c1-19(29-30-4)23-13-14-24-22-12-11-20-17-21(31-33(5,6)7)15

InchiKey: SUMPKNGBSGVILZ-QOMLESJASA-N

Formula: C28H51NO3Si2

SMILES: CON=C(C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]: 505.88

Physical Properties

Property code	Value	Unit	Source
logp	7.638		Crippen Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486252&Units=SI

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices