5.beta.-Pregnane-20-one-3.alpha.,21-diol, MO-TMS, # 1

Inchi: InChI=1S/C27H51NO3Si2/c1-27-16-15-22-21-12-10-20(31-33(6,7)8)17-19(21)9-11-23(22

InchiKey: NNRWPPWQIYJZFM-VCWMXXIDSA-N

Formula: C27H51NO3Si2

SMILES: CON=C(CO[Si](C)(C)C)[C@H]1CCC2C3CC[C@@H]4C[C@H](O[Si](C)(C)C)CCC4C3C

Mol. weight [g/mol]: 493.88

Physical Properties

Property code	Value	Unit	Source
logp	7.329		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R527081&Units=SI

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):

Legend

logp: Octanol/Water partition coefficient