5-«alpha»-Pregnan-3-«alpha»-ol, 20-«alpha»-GlcNAc, MeTMS

Inchi: InChI=1S/C41H81NO7Si4/c1-27(32-19-20-33-31-18-17-29-25-30(47-51(8,9)10)21-23-40

InchiKey: PBMNBRWQMVWHAT-ARERSMMKSA-N

Formula: C41H81NO7Si4

SMILES: CC(=O)NC1C(OC(C)C2CCC3C4CCC5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)OC(CO[S

Mol. weight [g/mol]: 812.43

Physical Properties

Property code	Value	Unit	Source
logp	9.792		Crippen Method
rinpol	4230.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393343&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):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices