5-Pregnen-3-«alpha»,20-«alpha»-diol-20-GlcNAc TMS

Inchi: InChI=1S/C41H79NO7Si4/c1-27(32-19-20-33-31-18-17-29-25-30(47-51(8,9)10)21-23-40

InchiKey: IHXNCGCWSBPANW-IVIGLZASSA-N

Formula: C41H79NO7Si4

SMILES: CC(=O)NC1C(OC(C)C2CCC3C4CC=C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)OC(CO[S

Mol. weight [g/mol]: 810.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	9.712		Crippen Method
rinpol	4383.00		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=R394237&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices