

5-«beta»-Pregnan-3-«alpha»,20-«alpha»-diol-20-GTMS, # 1

InChI=1S/C41H81NO7Si4/c1-27(32-19-20-33-31-18-17-29-25-30(47-51(8,9)10)21-23-40)PBMNBRWQMVWHAT-UONSOJNOSA-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	4201.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394168&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.cheméo.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

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<https://www.cheméo.com/cid/70-869-0/5-beta-Pregnan-3-alpha-20-alpha-diol-20-GlcNAc-TMS-1.pdf>

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