5-«beta»-Pregnan-3-«alpha»,20-«alpha»-diol-20-G
TMS, # 2

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-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	4230.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394173&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
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/71-159-7/5-beta-Pregnan-3-alpha-20-alpha-diol-20-GlcNAc-TMS-2.pdf
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