

5-«alpha»-Pregnan-3-«beta»-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-RPBCENISA-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
log10ws	-1.74		Crippen Method
logp	9.792		Crippen Method
rinpol	4325.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/58-559-8/5-alpha-Pregnan-3-beta-ol-20-alpha-GlcNAc-MeTMS.pdf>

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