Pregnan-2,3,20-triol, GlcNAc, MeTMS

Inchi: InChI=1S/C44H89NO8Si5/c1-29(48-42-39(45-30(2)46)41(53-58(17,18)19)40(52-57(14,1
InchiKey: DZSZRCHAOXSXMJ-HEOYEJPDSA-N
Formula: C44H89NO8Si5
SMILES: CC(=O)NC1C(OC(C)C2CCC3C4CCC5CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC5(C)C4CCC
Mol. weight [g/mol]: 900.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.24		Crippen Method
logp	10.622		Crippen Method
rinpol	4383.00		NIST Webbook
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=R393610&Units=SI

Legend

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

Latest version available from:
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