

5«beta»-Pregnan-3«alpha»,17«alpha»,21-triol-11,20-dione-MO-TMS

InChI: InChI=1S/C31H60N2O5Si3/c1-30-20-27(32-34-2)29-24-16-14-23(37-40(7,8)9)19-22(24)20-1
InChIKey: JDQMZSHPLOBGKD-RTHIJAESSA-N
Formula: C31H60N2O5Si3
SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2CCC3CC(O[Si](C)(C)C)C3
Mol. weight [g/mol]: 625.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.05		Crippen Method
logp	7.916		Crippen Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523485&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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