

3A,11B,17A,20A,21-Pentahydroxy-5B-pregnane,

tetrakis-TMS

InChI: InChI=1S/C33H68O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(34)4

InChIKey: BLFBPIZLLOGUJM-GYTMKSEBSA-N

Formula: C33H68O5Si4

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O)C(CO[Si](C)(C)C)C1

Mol. weight [g/mol]: 657.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.03		Crippen Method
logp	8.882		Crippen Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R108591&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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