

3A,17A,21-Trihydroxy-5B-pregnan-11,20-dione,

enol, tetrakis-TMS
InChI: InChI=1/C33H64O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)H4O5Si4
InChIKey: FFLDDWIKMXXSKB-NLFPBLEVSA-N

Formula: C33H64O5Si4
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(=O)CC2(C)C1CCC2(O[Si](C)(C)C)C(=CO[Si](C)(C)C)C
Mol. weight [g/mol]: 653.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.67		Crippen Method
logp	9.563		Crippen Method
rinpol	3112.00		NIST Webbook
rinpol	3112.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R108680&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/43-015-7/3A-17A-21-Trihydroxy-5B-pregnan-11-20-dione-enol-tetrakis-TMS.pdf>

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