

5-Pregnan-11-one, 3«alpha»,20«alpha»,21-trihydroxy, TMSO-TMS

Inchi: InChI=1S/C33H67NO4Si4/c1-32-20-19-25(36-40(6,7)8)21-24(32)15-16-26-27-17-18-28(3)
InchiKey: LSXMLVWRZGKOSX-QBMDPFLVSA-N
Formula: C33H67NO4Si4
SMILES: CC12CC(=NO[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(CO[Si](C)(C)C)C3
Mol. weight [g/mol]: 654.23

Physical Properties

Property code	Value	Unit	Source
logp	9.754		Crippen Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527274&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-528-1/5-Pregnan-11-one-3-alpha-20-alpha-21-trihydroxy-TMSO-TMS.pdf>

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