

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

Inchi: InChI=1S/C32H63NO4Si3/c1-13-34-33-28-21-32(3)26(16-17-27(32)29(37-40(10,11)12)2
InchiKey: QBSDTYMRXDFQEB-GMUYWZIDSA-N
Formula: C32H63NO4Si3
SMILES: CCON=C1CC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CC
Mol. weight [g/mol]: 610.10

Physical Properties

Property code	Value	Unit	Source
logp	8.939		Crippen Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527254&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-980-9/5-Pregnan-11-one-3-alpha-20-alpha-21-trihydroxy-EO-TMS.pdf>

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