

Silane, [(3«alpha»,5«beta»)-pregn-20-ene-3,17,20,21-tetra

Other names: 3,17,20,21-Tetrakis[(trimethylsilyl)oxy]-(3«alpha»,5«beta»)-pregn-20-ene
3B,17A,21-Trihydroxy-5B-pregnan-20-one, TMS

Inchi: InChI=1S/C33H66O4Si4/c1-31-20-17-26(35-39(6,7)8)23-25(31)15-16-27-28(31)18-21-32

InchiKey: YCSSNBJCYDGPCA-WBZRBYKWSA-N

Formula: C33H66O4Si4

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(=CO[Si](C)(C)C)C

Mol. weight [g/mol]: 639.22

CAS: 42599-94-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	10.384		Crippen Method
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C42599940&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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