

Silane, [(3«beta»,5«alpha»,11«beta»,17«alpha»,20R)-pregnane-3,11,17,20,21-pentaylpentakis(trimethylsilyloxy)]

Other names: Silane,
[(3«beta»,5«alpha»,11«beta»,17«alpha»,20R)-pregnane-3,11,17,20,21-pentaylpentakis(trimethylsilyloxy)]

Inchi: InChI=1S/C36H76O5Si5/c1-34-22-20-28(38-43(6,7)8)24-27(34)18-19-29-30-21-23-36(41-42)5-6

InchiKey: DUBRZSYNDDSLBA-CZPHMHNC-SA-N

Formula: C₃₆H₇₆O₅Si₅

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

Mol. weight [g/mol]: 729.41

CAS: 57456-94-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.84		Crippen Method
logp	10.741		Crippen Method
rinpol	3138.00		NIST Webbook
rinpol	3122.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	3122.00		NIST Webbook
rinpol	3122.00		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=C57456947&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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