Silane, [[(3«beta»,20S)-pregn-5-ene-3,20,21-triyl]tris(oxy)t

Other names: 5-Pregnene-3«beta»,20«beta»,21-triol, tris-TMS

Inchi: InChI=1S/C30H58O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30

InchiKey: RBSXFFWTNZTHKA-FPPZZAMFSA-N

Formula: C30H58O3Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC1

Mol. weight [g/mol]: 551.04

CAS: 57305-40-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	8.857		Crippen Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305405&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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