Silane, [[(3«alpha»,5«beta»,20S)-pregnane-3,17,20-triyl]tr

Other names: Silane, (5«beta»-pregnane-3«alpha»,17«alpha»,20«alpha»-triyltrioxy)tris[trimethyl-
Silane, (5«beta»-pregnane-3«alpha»,17,20«alpha»-triyltrioxy)tris[trimethyl-
3,17,20-Tris[(trimethylsilyl)oxy]pregnane, (3«alpha»,5«beta»,17«alpha»,20«alpha»)-
3«alpha»,17«alpha»,20«alpha»-Trihydroxy-5«beta»-pregnane, tris-TMS
3A,17A,20A-Trihydroxy-5B-pregnane, tris-TMS
Pregnane-3,17,20-triol, (3«alpha»,5«beta»,20s)-, 3tms derivative

Inchi: InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21

InchiKey: KFUWLVZCEDFJIK-UHFFFAOYSA-N

Formula: C30H60O3Si3

SMILES: CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 553.05

CAS: 17846-09-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	9.079		Crippen Method
rinpol	2818.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17846092&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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