allo-5B-Pregnan-3A,11B,21-triol-20-one, MO TMS

Inchi: InChI=1S/C31H61NO4Si3/c1-30-18-17-23(35-38(7,8)9)19-22(30)13-14-24-25-15-16-26(2

InchiKey: LTUTXXUPIPZWMI-DQGPTCKVSA-N

Formula: C31H61NO4Si3

SMILES: CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)C

Mol. weight [g/mol]: 596.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3030.00		NIST Webbook
rinpol	3011.00		NIST Webbook
rinpol	3030.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R104386&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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