5«beta»-Pregnane-3«alpha»,11«beta»,20«alpha»,2
EO-TMS

InchI: InChI=1S/C32H66O4Si4/c1-32-21-29(35-39(8,9)10)31-25-17-15-24(34-38(5,6)7)20-23(25
InchiKey: NLRITPVCQLIPHR-YNCGYUFOSA-N
Formula: C32H66O4Si4
SMILES: CC12CC(O[Si](C)(C)C)C3C4CCC(O[Si](C)(C)C)CC4CCC3C1CCC2C(CO[Si](C)(C)C)O[S
Mol. weight [g/mol]: 627.21

Physical Properties

Property code	Value	Unit	Source
log10ws	7.01e-03		Crippen Method
logp	9.377		Crippen Method
rinpol	3106.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3115.00		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=R527125&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
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