24-Nor-5«beta»-cholestane-3«alpha»,7«alpha»,25-triol-TMS

InChI: InChI=1S/C35H70O3Si3/c1-25(15-14-16-26(2)36-39(5,6)7)29-17-18-30-33-31(20-22-35(

InchiKey: FVPLBZWULCZECT-NEVZYZLOSA-N

Formula: C35H70O3Si3

SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)O[S

Mol. weight [g/mol]: 623.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	10.742		Crippen Method
rinpol	3339.00		NIST Webbook
rinpol	3339.00		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=R500140&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices