Methyl 5-«beta»-cholan-3-«alpha»-ol-7-one-24-oate, oxime, TMS

Inchi: InChI=1S/C31H57NO4Si2/c1-21(11-14-28(33)34-4)24-12-13-25-29-26(16-18-31(24,25)3
InchiKey: JIMAJZAKGBPGCN-MKOAOSGSSA-N
Formula: C31H57NO4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(=NO[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC1
Mol. weight [g/mol]: 563.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	8.272		Crippen Method
rinpol	3268.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R215946&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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