3-oxo-4-chol-24-oate, O-methyloxime-TMS (1)

Inchi: InChI=1S/C28H47NO3Si/c1-19(8-13-26(30)32-33(5,6)7)23-11-12-24-22-10-9-20-18-21(2
InchiKey: GJCWOGDLSUCAKE-BEVKLEDXSA-N
Formula: C28H47NO3Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCC(=O)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 473.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	7.362		Crippen Method
rinpol	3347.00		NIST Webbook
rinpol	3347.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492485&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