

Methyl chol-4-en-3-one-24-oate, oxime, TMS # 1

Inchi: InChI=1S/C28H47NO3Si/c1-19(8-13-26(30)31-4)23-11-12-24-22-10-9-20-18-21(29-32-33)25-27-28
InchiKey: XEAHYHSKAMKUDZ-ANYBSYGZSA-N
Formula: C28H47NO3Si
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4=CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 473.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	7.362		Crippen Method
rinpol	3335.00		NIST Webbook
rinpol	3337.00		NIST Webbook
rinpol	3335.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R216107&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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