

Methyl chol-4,6-dien-3-one-24-oate, oxime, TMS

Inchi: InChI=1S/C28H45NO3Si/c1-19(8-13-26(30)31-4)23-11-12-24-22-10-9-20-18-21(29-32-33)25-27-28-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: IORUVOSUGFPOIR-ANYBSYGZSA-N
Formula: C28H45NO3Si
SMILES: COC(=O)CCC(C)C1CCC2C3C=CC4=CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 471.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	7.138		Crippen Method
rinpol	3387.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R216063&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

Latest version available from:

<https://www.chemeo.com/cid/63-036-2/Methyl-chol-4-6-dien-3-one-24-oate-oxime-TMS.pdf>

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