

Methyl chol-4-en-3,7,12-trione-24-oate, oxime, TMS

Inchi: InChI=1S/C34H61N3O5Si3/c1-23(14-17-31(38)39-4)26-15-16-27-32-28(22-30(34(26,27)
InchiKey: YOGKVDANCQTORX-UHFFFAOYSA-N
Formula: C34H61N3O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(=NO[Si](C)(C)C)CC4=CC(=NO[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 676.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	8.997		Crippen Method
rinpol	3538.00		NIST Webbook
rinpol	3538.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R216083&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/20-382-5/Methyl-chol-4-en-3-7-12-trione-24-oate-oxime-TMS.pdf>

Generated by Cheméo on 2024-04-27 20:30:36.966172277 +0000 UTC m=+16539085.886749658.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.