

24-Ethyl-4,22-cholestadien-3-one, oxime, TMS # 1

Inchi: InChI=1S/C32H55NOSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-32)
InchiKey: OVTBSVUYAYIHMU-YYOOXWIVSA-N
Formula: C32H55NOSi
SMILES: CCC(C=CC(C)C1CCC2C3CCC4=CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 497.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.62		Crippen Method
logp	9.647		Crippen Method
rinpol	3395.00		NIST Webbook
rinpol	3395.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R215624&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/86-181-6/24-Ethyl-4-22-cholestadien-3-one-oxime-TMS-1.pdf>

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