24-Ethyl-5-«beta»-cholestan-3-one, oxime, TMS # 1

Inchi: InChI=1S/C32H59NOSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-

InchiKey: IICMQYRZGQRAFA-CMYCNLEQSA-N

Formula: C32H59NOSi

SMILES: CCC(CCC(C)C1CCC2C3CCC4CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C)C(C)C

Mol. weight [g/mol]: 501.90

Physical Properties

Property code	Value	Unit	Source
logp	9.951		Crippen Method
rinpol	3371.00		NIST Webbook
rinpol	3371.00		NIST Webbook
tf	371.62	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R215664&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point