

Methyl 5-.beta.-cholan-3-one-24-oate, oxime, TMS # 1

Inchi: InChI=1S/C28H49NO3Si/c1-19(8-13-26(30)31-4)23-11-12-24-22-10-9-20-18-21(29-32-33)25-27-28-26
InchiKey: NPBWLYGQYCAWNA-ILCQWMCYSA-N
Formula: C28H49NO3Si
SMILES: COC(=O)CCC(C)C1CCC2C3CC[C@@H]4C/C(=N\O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 475.79

Physical Properties

Property code	Value	Unit	Source
logp	7.442		Crippen Method
tf	385.33	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R215986>

Legend

logp: Octanol/Water partition coefficient
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/120-915-2/Methyl-5-beta-cholan-3-one-24-oate-oxime-TMS-1.pdf>

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