

Methyl 5-β-cholan-12-α-ol-3-one-24-oate, oxime, TMS # 2

InChI: CC(=O)OCCC(C)C1CCC2C3CC[C@@H]4C/C(=N/O[Si](C)(C)C)CCC4(C)C3C[C@H](O)C2
InChIKey: QIWSBVFPWMELCB-BNVKNMGISA-N
Formula: C₃₁H₅₇NO₄Si₂
SMILES: COC(=O)CCC(C)C1CCC2C3CC[C@@H]4C/C(=N/O[Si](C)(C)C)CCC4(C)C3C[C@H](O)C2
Mol. weight [g/mol]: 563.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Cheméo Relay (1.0)
logp	8.272		Crippen Method

Sources

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=R215788>
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

Latest version available from:

<https://www.chemeo.com/cid/120-958-5/Methyl-5-beta-cholan-12-alpha-ol-3-one-24-oate-oxime-TMS-2.pdf>

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