

Methyl 5-β-cholan-7-α-ol-3-one-24-oate, oxime, TMS #1

InChI: CC1=C(C(C(C(C1)C(=O)N=O)O[Si](C)(C)C)C[C@H]1C[C@H](C[C@@H]2[C@@H](C[C@H](C3=C(C(=O)O)CCC(C)C1CCC2C3C)C)C)C
InChIKey: CQTMZNGJGAEHPX-KZUUWTDGSA-N
Formula: C₃₁H₅₇NO₄Si₂
SMILES: COC(=O)CCC(C)C1CCC2C3C(CCC12C)C1(C)CC/C(=N/O[Si](C)(C)C)C[C@H]1C[C@H](C[C@@H]2[C@@H](C[C@H](C3=C(C(=O)O)CCC(C)C1CCC2C3C)C)C)C
Mol. weight [g/mol]: 563.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Cheméo Relay (1.0)
logp	8.272		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R216038>

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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/122-275-1/Methyl-5-beta-cholan-7-alpha-ol-3-one-24-oate-oxime-TMS-1.pdf>

Generated by Cheméo on 2026-07-21 13:42:42.412447864 +0000 UTC m=+152458.254333351.

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