4-Cholenoic acid, 7-«beta»-ol-3-one, TMS

Inchi: InChI=1S/C36H68O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36
InchiKey: GLKHZJHSPOOTGF-TXBBCWPISA-N
Formula: C36H68O5Si4
SMILES: C[C@H](CCC(=O)O[Si](C)(C)C)[C@H]1CCC2C3C(C[C@H](O[Si](C)(C)C)[C@@]21C)[C
Mol. weight [g/mol]: 693.28

Physical Properties

Property code	Value	Unit	Source
logp	10.365		Crippen Method
rinpol	3421.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177389&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):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/42-206-6/4-Cholenoic-acid-7-beta-ol-3-one-TMS.pdf
Generated by Cheméo on 2026-11-18 10:59:14.724795595 +0000 UTC m=+10035.939491169.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.