

3-«alpha»,7-«beta»,22-Trihydroxy-5-«beta»-cholic acid, methyl ester, TMS

InChI: InChI=1S/C34H66O5Si3/c1-23(29(22-31(35)36-4)38-41(8,9)10)26-14-15-27-32-28(17-19)OOEXXJOZTNHRHH-FPRKQBKWSA-N
InChIKey:
Formula: C34H66O5Si3
SMILES: COC(=O)CC(O[Si](C)(C)C)C(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3362.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393041&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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