Nordeoxycholic acid, trimethylsilyl ether-methyl ester

Inchi: InChI=1S/C30H56O4Si2/c1-20(17-28(31)32-4)24-13-14-25-23-12-11-21-18-22(33-35(5,6

InchiKey: NGPRYRMBFZRYLM-WTIROFSHSA-N

Formula: C30H56O4Si2

SMILES: COC(=O)CC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12C

Mol. weight [g/mol]: 536.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.895		Crippen Method
rinpol	3134.00		NIST Webbook

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=R182762&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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