

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/ci9903071>
Crippen Method: https://www.cheméo.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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