«DELTA»7-Lithocholic acid, trimethylsilyl ether-methyl ester

Other names: 3«alpha»-Hydroxy-«DELTA»7-5«beta» -cholanoic acid, MeTMS
Inchi: InChI=1S/C28H48O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)
InchiKey: WJIVWCYQOAJLNZ-UXUOZFMHSA-N
Formula: C28H48O3Si
SMILES: COC(=O)CCC(C)C1CCC2C3=CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 460.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	7.375		Crippen Method
rinpol	3177.00		NIST Webbook
rinpol	3186.00		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=R182262&Units=SI

Legend

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