3-«alpha»-Hydroxy-12-keto-5-«beta»-cholanoic acid, MeTMS

Inchi: InChI=1S/C28H48O4Si/c1-18(8-13-26(30)31-4)22-11-12-23-21-10-9-19-16-20(32-33(5,6)
InchiKey: AXQLYIJDHTZLNZ-GKONJBGUSA-N
Formula: C28H48O4Si
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(=O)C12C
Mol. weight [g/mol]: 476.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	6.634		Crippen Method

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=R393214&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

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