4,6-Choladienoic acid, 12-«alpha»-hydroxy-3-one, methyl ester, TMS

Other names: 12-«alpha»-Hydroxy-3-keto-4,6-choladienoic acid, MeTMS
Inchi: InChI=1S/C28H44O4Si/c1-18(8-13-26(30)31-4)22-11-12-23-21-10-9-19-16-20(29)14-15-
InchiKey: DXBZHLMBZSDCBW-NZOVMPDJSA-N
Formula: C28H44O4Si
SMILES: COC(=O)CCC(C)C1CCC2C3C=CC4=CC(=O)CCC4(C)C3CC(O[Si](C)(C)C)C12C
Mol. weight [g/mol]: 472.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	6.330		Crippen Method
rinpol	3335.00		NIST Webbook
rinpol	3335.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393110&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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