Cholanic acid, 3«alpha»-hydroxy, Me-TMS

Other names: 3«alpha»-Hydroxy-5«beta»-cholanic acid, methyl ester, TMS
Methyl 3-[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»)-
3«alpha»-Hydroxy-5«beta»-cholanoic acid, methyl ester, trimethylsilyl ether
3-«alpha»-Hydroxy-5-«beta»-cholanoic acid, methyl ester, TMS ether
5-«beta»-Cholanoic acid, 3-«alpha».-hydroxy, methyl ester, TMS
Lithocholic acid, trimethylsilyl ether, methyl ester
3«alpha»-hydroxy-5«beta»-cholanoic acid, MeTMS
Methyl lithocholate, (3«alpha»,5«beta»)-, tms derivative
Inchi: InChI=1S/C28H50O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)
InchiKey: MMCLGKIAEUXBCF-LHCCZRFYSA-N
Formula: C28H50O3Si
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 462.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	7.455		Crippen Method
rinpol	3141.00		NIST Webbook
rinpol	3103.00		NIST Webbook
rinpol	3133.00		NIST Webbook
rinpol	3179.00		NIST Webbook
rinpol	3157.00		NIST Webbook
rinpol	3141.00		NIST Webbook
rinpol	3103.00		NIST Webbook
rinpol	3133.00		NIST Webbook
rinpol	3179.00		NIST Webbook
rinpol	3103.00		NIST Webbook
ripol	3727.00		NIST Webbook
ripol	3647.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59953478&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices