allo-Cholanic acid, 12«alpha»-hydroxy, Me-TMS

Inchi: InChI=1S/C28H50O3Si/c1-19(11-16-26(29)30-4)22-14-15-23-21-13-12-20-10-8-9-17-27(

InchiKey: GVHHSUABUMNRNR-MNUIFVFYSA-N

Formula: C28H50O3Si

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CC(O[Si](C)(C)C)C12C

Mol. weight [g/mol]: 462.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Cheméo Relay (1.0)
logp	7.455		Crippen Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		NIST Webbook
ripol	3496.00		NIST Webbook
ripol	3496.00		NIST Webbook
tf	368.46	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533274&Units=SI

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices

tf: Normal melting (fusion) point