Cholanic acid, 3.alpha.,6.alpha.,7.alpha.-trihydroxy, Me-DMES

Inchi: InChI=1S/C37H72O5Si3/c1-14-43(8,9)40-27-21-23-37(6)30-22-24-36(5)28(26(4)17-20-3

InchiKey: NMKQJZYPICMVQH-YTWOWHBRSA-N

Formula: C37H72O5Si3

SMILES: CC[Si](C)(C)O[C@@H]1CC[C@@]2(C)[C@@H](C1)[C@@H](O[Si](C)(C)CC)[C@@H](

Mol. weight [g/mol]: 681.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Cheméo Relay (1.0)
logp	10.285		Crippen Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R533907

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