Cholanic acid, 3«alpha»,6«alpha»-dihydroxy, Me-DMES

Inchi: InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-24-17-19-33(5)28-18-20-32(4)26(23(3)13-16-3
InchiKey: GRDBFIKPYHWWBS-TZPPAOIUSA-N
Formula: C33H62O4Si2
SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)C(O[Si](C)(C)CC)CC1C3CCC(C(C)CCC(=O)OC)C3(C)C
Mol. weight [g/mol]: 579.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Cheméo Relay (1.0)
logp	9.065		Crippen Method
rinpol	3458.00		NIST Webbook
rinpol	3458.00		NIST Webbook
ripol	3668.00		NIST Webbook
ripol	3668.00		NIST Webbook
tf	374.60	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533927&Units=SI

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