

Cholanic acid, 7«beta»,12«alpha»-dihydroxy, Me-DMES

Inchi: InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-28-21-24-15-13-14-20-32(24,4)27-22-29(37-39)23-30-31
InchiKey: CEXBTJDTURZYOY-UTKSZCFKSA-N
Formula: C33H62O4Si2
SMILES: CC[Si](C)(C)OC1CC2CCCCC2(C)C2CC(O[Si](C)(C)CC)C3(C)C(C(C)CCC(=O)OC)CCC
Mol. weight [g/mol]: 579.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3328.00		NIST Webbook
rinpol	3328.00		NIST Webbook
ripol	3681.00		NIST Webbook
ripol	3681.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534326&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

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