

Cholanic acid, 3«beta»,7«beta»,12«alpha»-trihydroxy, Me-DMES

InChI: InChI=1S/C37H72O5Si3/c1-14-43(8,9)40-28-21-22-36(5)27(23-28)24-32(41-44(10,11)15
InChIKey: QIHGNFRQNAWOFU-BTFJHGPGSA-N
Formula: C37H72O5Si3
SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CC(O[Si](C)(C)CC)C2(C)C(C(C
Mol. weight [g/mol]: 681.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	10.285		Crippen Method
rinpol	3552.00		NIST Webbook
rinpol	3552.00		NIST Webbook
ripol	3815.00		NIST Webbook
ripol	3815.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534188&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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