

3«alpha»-hydroxy-5«beta»-cholan-24-oic acid, DMESI

Inchi:	InChI=1S/C32H60O3Si2/c1-10-36(6,7)34-25-18-20-31(4)24(22-25)13-14-26-28-16-15-27
InchiKey:	SIZVXIMNEHZJBV-KVHLQNDXSA-N
Formula:	C32H60O3Si2
SMILES:	CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)CC)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	548.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	9.440		Crippen Method
rinpol	3321.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R279980&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/56-144-0/3-alpha-hydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf>

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