

allo-Cholanic acid, 7«alpha»-hydroxy, Me-DMES

Inchi:	InChI=1S/C29H52O3Si/c1-8-33(6,7)32-25-19-21-11-9-10-17-28(21,3)24-16-18-29(4)22(1)
InchiKey:	RKNVOTKYHVSSQK-IZRCTVDGSA-N
Formula:	C29H52O3Si
SMILES:	CC[Si](C)(C)OC1CC2CCCCC2(C)C2CCC3(C)C(C(C)CCC(=O)OC)CCC3C12
Mol. weight [g/mol]:	476.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	7.845		Crippen Method
rinpol	3106.00		NIST Webbook
ripol	3540.00		NIST Webbook
ripol	3540.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533749&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

Latest version available from:

<https://www.chemeo.com/cid/70-209-2/allo-Cholanic-acid-7-alpha-hydroxy-Me-DMES.pdf>

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