

allo-Cholanic acid, 12«alpha»-hydroxy, Me-DMES

Inchi:	InChI=1S/C29H52O3Si/c1-8-33(6,7)32-26-19-25-22(14-13-21-11-9-10-18-28(21,25)3)24
InchiKey:	DBDZGEARTPZCLG-GQPOEMMZSA-N
Formula:	C29H52O3Si
SMILES:	CC[Si](C)(C)OC1CC2C(CCC3CCCCC32C)C2CCC(C(C)CCC(=O)OC)C12C
Mol. weight [g/mol]:	476.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	7.845		Crippen Method
rinpol	3118.00		NIST Webbook
ripol	3580.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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<https://www.chemeo.com/cid/21-017-9/allo-Cholanic-acid-12-alpha-hydroxy-Me-DMES.pdf>

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