

allo-Cholanic acid, 12«beta»-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-HCOBZBMTSA-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	3132.00		NIST Webbook
rinpol	3132.00		NIST Webbook
ripol	3580.00		NIST Webbook
ripol	3580.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533289&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

Latest version available from:

<https://www.cheméo.com/cid/11-256-5/allo-Cholanic-acid-12-beta-hydroxy-Me-DMES.pdf>

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