

1 «beta»,2 «beta»-Epoxy-7-hydroxy-1 «alpha»-meth

Inchi:	InChI=1S/C9H15NO3/c1-12-5-9-7(13-9)4-10-3-2-6(11)8(9)10/h6-8,11H,2-5H2,1H3/t6?,7?
InchiKey:	BYURGVBM CJUJQD-UYXKVS BOSA-N
Formula:	C9H15NO3
SMILES:	COCC12OC1CN1CCC(O)C12
Mol. weight [g/mol]:	185.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	-0.781		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
rmpol	1460.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R590202&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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