

Littorine

Inchi:	InChI=1S/C17H23NO3/c1-18-13-7-8-14(18)11-15(10-13)21-17(20)16(19)9-12-5-3-2-4-6-
InchiKey:	FNRXUEYLFZLOEZ-UHFFFAOYSA-N
Formula:	C17H23NO3
SMILES:	CN1C2CCC1CC(OC(=O)C(O)Cc1cccc1)C2
Mol. weight [g/mol]:	289.37
CAS:	21956-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	1.758		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
rinpol	2601.20		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21956478&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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/13-222-0/Littorine.pdf>

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