

6-Hydroxylittorine

Inchi: InChI=1S/C17H23NO4/c1-18-12-8-13(10-14(18)15(19)9-12)22-17(21)16(20)7-11-5-3-2-4
InchiKey: HJHAFGCQRMACPE-UHFFFAOYSA-N
Formula: C17H23NO4
SMILES: CN1C2CC(OC(=O)C(O)Cc3ccccc3)CC1C(O)C2
Mol. weight [g/mol]: 305.37
CAS: 137198-36-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	0.729		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
rinpol	2972.50		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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=C137198368&Units=SI>

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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