Betameprodine

Inchi: InChI=1S/C17H25NO2/c1-4-14-13-18(3)12-11-17(14,20-16(19)5-2)15-9-7-6-8-10-15/h6-1
InchiKey: ODEGQXRCQDVXSJ-UHFFFAOYSA-N
Formula: C17H25NO2
SMILES: CCC(=O)OC1(c2ccccc2)CCN(C)CC1CC
Mol. weight [g/mol]: 275.39
CAS: 468-50-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	3.197		Crippen Method
mcvol	233.190	ml/mol	McGowan Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C468508&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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