Remoxipride

Other names:	Benzamide, 3-bromo-2,6-dimethoxy-N-(1-ethyl-2-pyrrolidinylmethyl)-, hydrochloride, (S)-(-)- (S)-(-)-2-((3-Bromo-2,6-dimethoxybenzamido)methyl)-1-ethylpyrrolidine hydrochloride (S)-(-)-3-Bromo-2,6-dimethoxy-N-(1-ethyl-2-pyrrolidinylmethyl)benzamide hydrochloride Benzamide, 3-bromo-N-[(1-ethyl-2-pyrrolidinyl)methyl]-2,6-dimethoxy-, (S)- ((-))-(S)-3-Bromo-N-[(1-ethyl-2-pyrrolidinyl)methyl]-2,6-dimethoxybenzamide
Inchi:	InChI=1S/C16H23BrN2O3/c1-4-19-9-5-6-11(19)10-18-16(20)14-13(21-2)8-7-12(17)15(14
InchiKey:	GUJRSXAPGDDABA-UHFFFAOYSA-N
Formula:	C16H23BrN2O3
SMILES:	CCN1CCCC1CNC(=O)c1c(OC)ccc(Br)c1OC
Mol. weight [g/mol]:	371.27
CAS:	80125-14-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	2.680		Crippen Method
mcvol	252.450	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80125140&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume