Moclobemide

Other names:	Benzamide, 4-chloro-N-(2-(4-morpholinyl)ethyl)-
	4-Chloro-N-(2-(4-morpholinyl)ethyl)benzamide
	RO 11-1163
	p-Chloro-N-(2-morpholinoethyl)benzamide
	Aurorix
	Manerix
	Moclaime
	Moclamide
	Ro-11-1163/000
	Auromid
Inchi:	InChI=1S/C13H17ClN2O2/c14-12-3-1-11(2-4-12)13(17)15-5-6-16-7-9-18-10-8-16/h1-4H,
InchiKey:	YHXISWVBGDMDLQ-UHFFFAOYSA-N
Formula:	C13H17ClN2O2
SMILES:	O=C(NCCN1CCOCC1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	268.74
CAS:	71320-77-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	1.402		Crippen Method
mcvol	199.050	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook

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=C71320779&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