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

Physical Properties

Property code	Value	Unit	Source
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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71320779&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices