Meclizine

Other names:

(.+/-.)-Meclizine
1-(p-Chloro-«alpha»-phenylbenzyl)-4-(m-methylbenzyl)piperazine
1-(p-Chloro-Â«alphaÂ»-phenylbenzyl)-4-(m-methylbenzyl)piperazine
1-(p-Chlorobenzhydryl)-4-(m-methylbenzyl)diethylenediamine
1-(p-Chlorobenzhydryl)-4-(m-methylbenzyl)piperazine
1-[(4-chlorophenyl)-phenylmethyl]-4-[(3-methylphenyl)methyl]piperazine
Ancolan
Ancolon
Antivert
Bonadettes
Bonine
Calmonal
Chiclida
Histamethine
Histamethizine
Histametizine
Histametizyne
Itinerol
Marex
Meclozine
Monamine
NSC 169189
Navicalm
Neo-Istafene
Parachloramine
Peremesin
Piperazine, 1-(p-chloro-alpha-phenylbenzyl)-4-(m-methylbenzyl)-
Piperazine, 1-(p-chloro-«alpha»-phenylbenzyl)-4-(m-methylbenzyl)-
Piperazine, 1-(p-chloro-Â«alphaÂ»-phenylbenzyl)-4-(m-methylbenzyl)-
Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-[(3-methylphenyl)methyl]-
Postafen
Postafene
Ravelon
Sabari
Sea-Legs
Siguran
Suprimal
Travelon
U. C. B. 5062
UCB 5052

UCB 5062
Vibazine
Vomisseis
Vomissels
neo-Suprimal
neo-Suprimel

Inchi: InChI=1S/C25H27ClN2/c1-20-6-5-7-21(18-20)19-27-14-16-28(17-15-27)25(22-8-3-2-4-9-

InchiKey: OCJYIGYOJCODJL-UHFFFAOYSA-N

Formula: C25H27ClN2

SMILES: Cc1cccc(CN2CCN(C(c3ccccc3)c3ccc(Cl)cc3)CC2)c1

Mol. weight [g/mol]: 390.95

CAS: 569-65-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Aqueous Solubility Prediction Method
logp	5.556		Crippen Method
mcvol	313.170	ml/mol	McGowan Method
rinpol	3040.00		NIST Webbook
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
rinpol	3000.00		NIST Webbook
rinpol	3040.00		NIST Webbook
rinpol	3050.00		NIST Webbook
rinpol	3035.00		NIST Webbook
rinpol	3033.00		NIST Webbook
rinpol	3050.00		NIST Webbook
rinpol	3033.00		NIST Webbook
rinpol	3040.00		NIST Webbook
rinpol	3030.00		NIST Webbook
rinpol	3034.00		NIST Webbook
rinpol	3040.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C569653&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