

Chlorcyclizine

Other names:

Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-methyl-
Piperazine, 1-(p-chloro-«alpha»-phenylbenzyl)-4-methyl-
Alergicide
Chlorcycline
Chlorocycline
Chlorocyclizine
Compound 47-282
Di-paralen
Di-paralene
N-Methyl-N'-(4-chlorobenzhydryl)piperazine
Perazyl
Trihistan
1-(p-Chloro-«alpha»-phenylbenzyl)-4-methylpiperazine
1-(4-Chlorobenzhydryl)-4-methylpiperazine
1-[(4-Chlorophenyl)phenylmethyl]-4-methylpiperazine
Histantin
Histantine
NSC 25246

Inchi:

InChI=1S/C18H21ClN2/c1-20-11-13-21(14-12-20)18(15-5-3-2-4-6-15)16-7-9-17(19)10-8

InchiKey:

WFNAKBGANONZEQ-UHFFFAOYSA-N

Formula:

C18H21ClN2

SMILES:

CN1CCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1

Mol. weight [g/mol]:

300.83

CAS:

82-93-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.677		Crippen Method
mcpol	238.300	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2225.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C82939&Units=SI

Legend

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

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