

Clemizole

Other names:

1H-Benzimidazole, 1-[(4-chlorophenyl)methyl]-2-(1-pyrrolidinylmethyl)-
Benzimidazole, 1-(p-chlorobenzyl)-2-(1-pyrrolidinylmethyl)-
Clemizol
Histacur
Histakool
1-(p-Chlorobenzyl)-2-pyrrolidylmethylenbenzimidazole
1-p-Chlorobenzyl-2-(1-pyrrolidinylmethyl)benzimidazole
1-[(4-Chlorophenyl)methyl]-2-(1-pyrrolidinylmethyl)-1H-benzimidazole
Depocural
Lergopenin
NSC 46261

Inchi:

Pyrrolidine, 1-[(1-p-chlorobenzyl-2-benzimidazolyl)methyl]-
InChI=1S/C19H20ClN3/c20-16-9-7-15(8-10-16)13-23-18-6-2-1-5-17(18)21-19(23)14-22-

InchiKey:

CJXAEXPPLWQRFR-UHFFFAOYSA-N

Formula:

C19H20ClN3

SMILES:

Clc1ccc(Cn2c(CN3CCCC3)nc3ccccc32)cc1

Mol. weight [g/mol]:

325.83

CAS:

442-52-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	4.334		Crippen Method
mcvol	247.210	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2620.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C442524&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

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