

# Clothiapine

**Other names:**

Dibenzo[b,f][1,4]thiazepine, 2-chloro-11-(4-methyl-1-piperazinyl)-  
2-Chloro-11-(4-methylpiperazino)dibenzo(b,f)(1,4)thiazepine  
2-Chloro-11-(4-methyl-1-piperazinyl)dibenzo(b,f)(1,4)thiazepine  
Clotiapine  
Entumin  
Etumine  
HF 2159  
LW 2159  
S-805C  
Entumine

**Inchi:**

InChI=1S/C18H18ClN3S/c1-21-8-10-22(11-9-21)18-14-12-13(19)6-7-16(14)23-17-5-3-2-

**InchiKey:**

KAAZGXDPUNNEFN-UHFFFAOYSA-N

**Formula:**

C18H18ClN3S

**SMILES:**

CN1CCN(C2=Nc3cccc3Sc3ccc(Cl)cc32)CC1

**Mol. weight [g/mol]:**

343.87

**CAS:**

2058-52-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	4.130		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
rinpole	2710.00		NIST Webbook
rinpole	2683.00		NIST Webbook
rinpole	2705.00		NIST Webbook

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2058528&Units=SI>

**Crippen Method:**

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

**Crippen Method:**

[https://www.chemed.com/doc/models/crippen\\_log10ws](https://www.chemed.com/doc/models/crippen_log10ws)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

# Legend

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

Latest version available from:

<https://www.cheméo.com/cid/99-250-5/Clothiapine.pdf>

Generated by Cheméo on 2024-04-24 09:39:36.100607646 +0000 UTC m=+16240825.021184961.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.