

Chlorpromazine  
hydrochloride  
C17H20Cl2N2S  
structure



**ASSIGN  
BUSTER**

## Contents

- Bio Activity:

Molecular      C<sub>17</sub> H<sub>20</sub> Cl<sub>2</sub> N<sub>2</sub>

Formula        S

Average mass   355. 325 Da

Density

Boiling Point

Flash Point

Molar

Refractivity

Polarizability

Surface Tension

Molar Volume

- Experimental data
- Predicted - ACD/Labs
- Predicted - ChemAxon
- Predicted - Mcule
  
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

197 °C  
CTCIC2481

193 °C

(Decomposes)  
Oxford

University Chemical

Safety Data (No longer

updated)  
More details

179 °C

(Decomposes)  
LKT

Labs[C2947]

195 °C  
BiosynthQ-

200843

196-198

°C  
LabNetworkLN001595

40

- **Experimental Flash Point:**

226 °C  
BiosynthQ-

200843

- **Experimental Gravity:**

226 g/mL  
BiosynthQ-

200843

- **Experimental Solubility:**

DMSO 72 mg/mL; Water

70 mg/mL MedChem

Express [http://www.medchemexpress.com/clindamycin-](http://www.medchemexpress.com/clindamycin-hydrochloride.html)

hydrochloride.html, HY-

B0407A

DMSO: 25 mg/ml ;

ethanol: 10 mg/ml;

water: < 0.1 mg/ml;

chloroform MedChem

Express HY-B0407A

Soluble in methanol,

ethanol, chloroform or

water. Insoluble in ether,

or benzene. LKT

Labs [C2947]

Labs [C2947]

Labs [C2947]

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

197 °C

197

°CTCIC2481

- Miscellaneous

- **Appearance:**

creamy white crystalline

powderOxford University

Chemical Safety Data

(No longer updated)More

details

- **Stability:**

Stable. Combustible.

Incompatible with strong

oxidizing agents. Air and

light sesnsitive. Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Toxicity:**

IPR-RAT LD50 62 mg kg-

1, SCU-RAT LD50 140

mg kg-1, IVN-RAT LD50

25 mg kg<sup>-1</sup>, ORL-RAT  
LD50 145 mg kg<sup>-1</sup>, IVN-  
RBT LD50 5 mg kg<sup>-1</sup>  
1Oxford University  
Chemical Safety Data  
(No longer updated)More  
details

- **Safety:**

25-26LKT Labs[C2947]

DangerBiosynthQ-

200843

GHS06BiosynthQ-

200843

H301 H330LKT

Labs[C2947]

H301; H330BiosynthQ-

200843

IRRITANTMatrix

Scientific058317

P260; P284; P301+P310;

P310BiosynthQ-200843

Safety glasses, good

ventilation. Gloves.

Oxford University

Chemical Safety Data

(No longer updated)More

details

T+Abblis

ChemicalsAB1009377

T+LKT Labs[C2947]

UN 2811 6. 1/PG 1LKT

Labs[C2947]

- **Target Organs:**

Histamine Receptor

antagonist; Potassium

Channel inhibitor;

Dopamine Receptor

antagonist; Adrenergic

Receptor antagonist;

AChR antagonist; 5-HT

receptor

antagonistTargetMolT13

84

- **Bio Activity:**

Calcium Channel

Dopamine

ReceptorMedChem

ExpressHY-B0407A

Chlorpromazine

Hydrochloride is a

dopamine and

potassium channel

inhibitor used as the

prototypical

phenothiazine

antipsychotic drug.

MedChem

Express[http://www.](http://www.medchemexpress.com/clindamycin-hydrochloride.html)

medchemexpress.

com/clindamycin-

hydrochloride. html, HY-

B0407A

Chlorpromazine

Hydrochloride is a

dopamine and



potassium channel  
inhibitor used as the  
prototypical  
phenothiazine  
antipsychotic drug. ;  
Target: Potassium  
Channel; Dopamine  
ReceptorChlorpromazine  
is a dopamine  
antagonist of the typical  
antipsychotic class of  
medications possessing  
additional  
antiadrenergic,  
antiserotonergic,  
anticholinergic and  
antihistaminergic  
properties used to treat  
schizophrenia.

Chlorpromazine works  
on a variety of receptors  
in the central nervous  
system [1, 2]. MedChem  
ExpressHY-B0407A

Dopamine

ReceptorMedChem

ExpressHY-B0407A

GPCR/G

proteinMedChem

ExpressHY-B0407A

GPCR/G protein;

Membrane

Tranporter/Ion Channel;

Neuronal Signaling;

MedChem ExpressHY-

B0407A

Histamine H1 receptor;

Potassium Channel ;

Dopamine receptor;

Adrenergic receptor;

Muscarinic AChR; 5-HT

receptorTargetMolT1384

NeuroscienceTargetMolT

1384

Predicted data is generated using the ACD/Labs Percepta Platform -  
PhysChem Module

No predicted properties have been calculated for this compound.

<https://assignbuster.com/chlorpromazine-hydrochloride-c17h20cl2n2s-structure/>

Density:

Boiling Point:

Vapour Pressure:

Enthalpy of Vaporization:

Flash Point:

Index of Refraction:

Molar Refractivity:

#H bond acceptors:

#H bond donors:

#Freely Rotating Bonds:

#Rule of 5 Violations:

ACD/LogP:

ACD/LogD (pH 5.5):

ACD/BCF (pH 5.5):

ACD/KOC (pH 5.5):

ACD/LogD (pH 7.4):

ACD/BCF (pH 7.4):

ACD/KOC (pH 7.4):

Polar Surface Area:

Polarizability:

Surface Tension:

Molar Volume:

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop