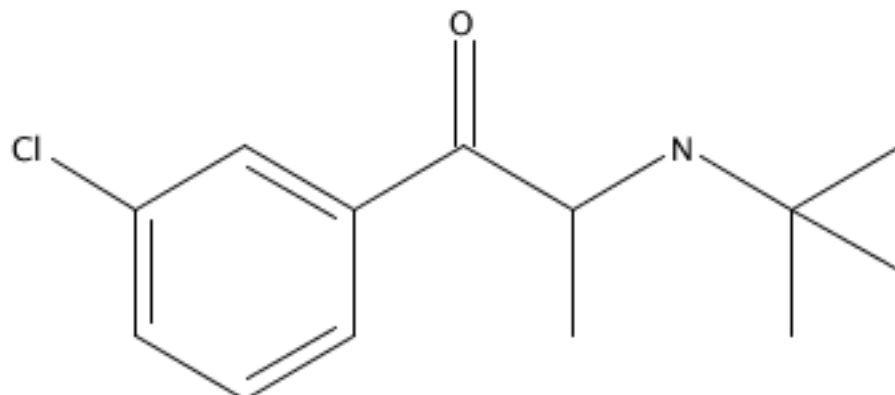


Task History

Task Began May 13, 2020 12:28 PM

Explore substances by SIMILARITY_2D_EXACT



Candidates: 9

Candidates Selected (ID 7)

Answer Type: 99 (most similar)

Result Count: Substances

114

Detailed display

From ID: 7

Type: 31677-93-7

CAS Registry Number: 31677-93-7

(Component: 34911-55-2)

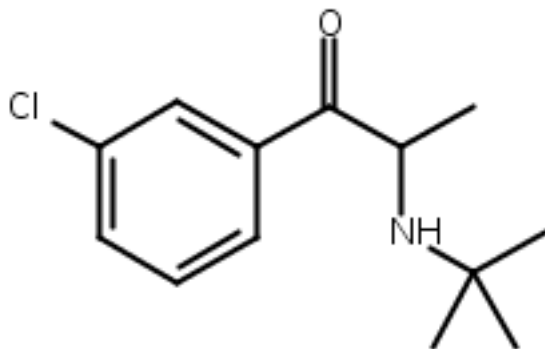
C₁₃ H₁₈ Cl N O · Cl H

1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride (1:1)

Melting Point (Experimental)

Value: 233-234 °C

Other Names: 1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride (9Cl); 1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride, (±)-; Propiophenone, 2-(*tert*-butylamino)-3'-chloro-, hydrochloride, (±)- (8Cl); Bupropion hydrochloride; DL- α -*t*-butylamino-3-chloropropiophenone hydrochloride; NSC 315851; Wellbatrin; Wellbutrin; Zyban; Zyban (pharmaceutical); *m*-Chloro- α -*tert*-butylaminopropiophenone hydrochloride; α -(*tert*-Butylamino)-*m*-chloropropiophenone hydrochloride

Deleted CAS Registry Numbers: 34841-36-6

● HCl

~612 References

~127 Commercial Sources

Experimental Properties: Biological Spectra Structure Related Thermal

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(1)CAS
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(2)CAS
Half-Life (Biological)	See full text		(2)CAS
Median Lethal Dose(LD50)	600 mg/kg	Organism: rat Route: oral	(8)APC
Median Lethal Dose(LD50)	575 mg/kg	Organism: mouse Route: oral	(8)APC
Median Lethal Dose(LD50)	230 mg/kg	Organism: mouse Route: intraperitoneal	(8)APC
Median Lethal Dose(LD50)	210 mg/kg	Organism: rat Route: intraperitoneal	(8)APC
Structure Related Properties	Value	Condition	Note
Crystal Structure	See full text		(5)CAS
Molecular Structure	See full text		(5)CAS
X-Ray Diffraction Pattern	See full text		(5)CAS
Thermal Properties	Value	Condition	Note
Melting Point	236-238 °C	Solv: ethyl ether (60-29-7)	(4)CAS
Melting Point	233-234 °C		(3)CAS
Melting Point	233-234 °C		(8)APC
Melting Point	233-234 °C		(9)NLM
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See full text		(3)CAS
Carbon-13 NMR Spectrum	See full text		(4)CAS
IR Absorption Spectrum	See spectrum		(6)BIORAD
Mass Spectrum	See spectrum		(7)WSS

Proton NMR Spectrum See full text
Proton NMR Spectrum See full text

(4)CAS
(3)CAS

- (1) Midha, K. K.; International Journal of Clinical Pharmacology and Therapeutics 2005, V43(5), P244-254 CAPLUS
- (2) Wen, Yuguan; Zhongguo Yiyuan Yaoxue Zazhi 2004, V24(7), P399-400 CAPLUS
- (3) Reddy, Y. Thirupathi; Synthetic Communications 2010, V40(11), P1566-1573 CAPLUS
- (4) Hamad, Mohamed O.; Bioorganic & Medicinal Chemistry 2006, V14(20), P7051-7061 CAPLUS
- (5) Vladiskovic, Chiara; Crystal Growth & Design 2014, V14(7), P3603-3611 CAPLUS
- (6) BIORAD: Infrared spectral data from the Bio-Rad/Sadtler IR Data Collection was obtained from Bio-Rad Laboratories, Philadelphia, PA (US).
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- (7) WSS: Spectral data were obtained from Wiley Subscription Services, Inc. (US)
- (8) "Drugs - Synonyms and Properties" data were obtained from Ashgate Publishing Co. (US)
- (9) "Hazardous Substances Data Bank" data were obtained from the National Library of Medicine (US)

REGULATORY INFORMATION :

Regulatory Synonyms

(±)-2-(tert-butylamino)-3'-chloropropiophenone hydrochloride (REACH, EINECS)
(±)-2-(tert-butylamino)-3'-chloropropiophenone, chlorhydrate (French) (EINECS)
(±)-2-(tert-Butylamino)-3'-chloropropiophenonhydrochlorid (German) (EINECS)
(±)-2-(terc-butilamino)-3'-cloropropiopenona, clorhidrato (Spanish) (EINECS)
1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride (1:1) (TCSI, INSQ)
1-propanona, 1-(3-clorofenil)-2-[(1,1-dimetiletil)amino]-, clorhidrato (1:1) (Spanish) (INSQ)
1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride
1-Propanone, 1-(3-chlorophenyl)-2-[(1,1-dimethylethyl)amino]-, hydrochloride, (±)-
Propiophenone, 2-(tert-butylamino)-3'-chloro-, hydrochloride, (±)-
α-(tert-Butylamino)-m-chloropropiophenone hydrochloride
2-(tert-butylamino)-1-(3-chlorophenyl)propan-1-one hydrochloride
bupropion hydrochloride
DL-α-t-Butylamino-3-chloropropiophenone hydrochloride
m-Chloro-α-tert-butylaminopropiophenone hydrochloride
NSC 315851
Wellbatrin
Wellbutrin
Zyban
Zyban (pharmaceutical)

Regulatory Overview by Country

Confidentiality Status

Public

European Union

EU Customs Code CN:

29223900

Inventory Status

On REACH

List of Pre-Registered Substances, March 2009

Registration Date: 30-NOV-2010.

On EINECS

Annex to Official Journal of the European Communities, 15 June 1990

Regulatory List Number

EC No.: 250-759-9

EINECS No.: 250-759-9

Mexico**Inventory Status**

On INSQ

National Inventory of Chemical Substances in Mexico, 2012

International and other lists**Harmonized Tariff Code**

292239

Inventory Status

On TCSI

Taiwan Government Gazette, 2015

Regulatory Inventories**File Segment**

EEC: EINECS

EU: REACH

Harmonized Tariff Code: HTC

MEXICO: INSQ

TAIWAN: TCSI

Bioactivity Indicators		References		
Nervous system agents (all) >>>> Antidepressants		151		
Nervous system agents (all) >>>> Antipsychotics		55		
Nervous system agents (all) >>>> Antipsychotics		55		
Target Indicators		References		
Proteins (all) >>>>> Cytochrome P450 CYP2B6		14		
Proteins (all) >>>>> Cytochrome P450 CYP2B6		14		
Proteins (all) >>>>> Cytochrome P450 CYP2B6		14		
Proteins (all) >>>> Cytochrome P450 CYP2B6		14		
Proteins (all) >>>> Monoamine oxidase		14		
CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓		
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative		✓		
Occurrence		✓		

Preparation	✓	✓	✓
Process	✓	✓	✓
Properties	✓	✓	✓
Reactant or Reagent	✓	✓	✓
Uses	✓	✓	✓

Document Type(s): Book, Conference, Journal, Patent

Source of Registration: CA