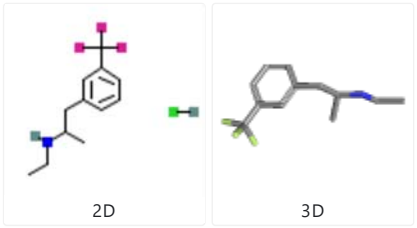
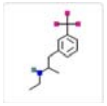
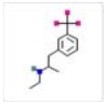
PubChem **REVIEWED**
**By Chris at 9:39 am, Mar 03, 2020**

COMPOUND SUMMARY

# Fenfluramine hydrochloride

| | |
|---|---|
| PubChem CID: | 91452 |
| Structure: |  2D 3D<br>Find Similar Structures |
| Chemical Safety: |  Acute Toxic Irritant<br>Laboratory Chemical Safety Summary (LCSS) Datasheet |
| Molecular Formula: | $C_{12}H_{17}ClF_3N$ |
| Synonyms: | Fenfluramine hydrochloride<br>Ponderal<br>Ponderax<br>Pondimin<br>Ganal<br>More... |
| Molecular Weight: | 267.72 g/mol |
| Parent Compound: |  CID 3337 (Fenfluramine) |
| Component Compounds: |  CID 3337 (Fenfluramine)<br> CID 313 (Hydrochloric acid) |
| Dates: | Modify: 2020-02-29 Create: 2005-08-08 |

Fenfluramine Hydrochloride is the hydrochloride salt of fenfluramine, an amphetamine derivative and a sympathomimetic stimulant with appetite-suppressant properties. Fenfluramine, which was part of the Fen-Phen anti-obesity medication, stimulates the release of serotonin from vesicular storage, and modulates serotonin transporter

function. Since serotonin regulates mood and appetite, among other functions, increased serotonin level results in a feeling of fullness and loss of appetite.

- NCI Thesaurus (NCIt)

A centrally active drug that apparently both blocks serotonin uptake and provokes transport-mediated serotonin release.

- MeSH

# 1 Structures

## 1.1 2D Structure

Chemical Structure Depiction


PubChem

## 1.2 3D Conformer

3D Conformer of Parent

PubChem

# 2 Names and Identifiers

## 2.1 Computed Descriptors

### 2.1.1 IUPAC Name

*N*-ethyl-1-[3-(trifluoromethyl)phenyl]propan-2-amine;hydrochloride

*Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)*

PubChem

### 2.1.2 InChI

InChI=1S/C12H16F3N.ClH/c1-3-16-9(2)7-10-5-4-6-11(8-10)12(13,14)15;/h4-6,8-9,16H,3,7H2,1-2H3;1H

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

PubChem

### 2.1.3 InChI Key

ZXKXJHAOUFHNAS-UHFFFAOYSA-N

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

PubChem

### 2.1.4 Canonical SMILES

CCNC(C)CC1=CC(=CC=C1)C(F)(F)F.Cl

*Computed by OEChem 2.1.5 (PubChem release 2019.06.18)*

PubChem

## 2.2 Molecular Formula

$C_{12}H_{17}ClF_3N$

*Computed by PubChem 2.1 (PubChem release 2019.06.18)*

PubChem

## 2.3 Other Identifiers

### 2.3.1 CAS

404-82-0

ChemIDplus; European Chemicals Agency (ECHA)

Related CAS

458-24-2 (Parent)

- ChemIDplus

### 2.3.1 Other CAS

16105-77-4

- ChemIDplus

### 2.3.2 European Community (EC) Number

206-968-2

- European Chemicals Agency (ECHA)

### 2.3.3 Wikipedia

Fenfluramine hydrochloride

- Wikipedia

## 2.4 Synonyms

### 2.4.1 MeSH Entry Terms

Fenfluramine
Fenfluramine Hydrochloride
Fenfluramine Hydrochloride, (+-)-Isomer
Fenfluramine Hydrochloride, R Isomer
Fenfluramine Hydrochloride, R-Isomer
Fenfluramine, (+-)-Isomer
Fenfluramine, R Isomer
Fenfluramine, R-Isomer
Hydrochloride, Fenfluramine
Isomeride
Pondimin

- MeSH

### 2.4.2 Depositor-Supplied Synonyms

| | | |
|---|---|---|
| Fenfluramine hydrochloride | AHR 3002 | Benzeneethan |
| Ponderal | EINECS 206-968-2 | Phenethylamir |
| Ponderax | AHR-3002 | Phenethylamir |
| Pondimin | Fenfluramin | CHEBI:59729 |
| Ganal | DEA No. 1670 | C12H16F3N.H |
| Fenfluramine HCl | 1-(3-Trifluoromethylphenyl)-2-ethylaminopropane hydrochloride | dl-Fenfluramir |
| 404-82-0 | N-ethyl-1-[3-(trifluoromethyl)phenyl]propan-2-amine hydrochloride | N-ethyl-1-[3-( |
| 16105-77-4 | N-Ethyl-alpha-methyl-3-trifluoromethylphenethylamine hydrochloride | ZX008 |
| Phenfluoramine hydrochloride | N-Ethyl-alpha-methyl-m-(trifluoromethyl)phenethylamine hydrochloride | Pondimin (TN) |
| (+-)-Fenfluramine chloride | N-ETHYL-1-(3-(TRIFLUOROMETHYL)PHENYL)PROPAN-2-AMINE HYDROCHLORIDE | SCHEMBL3949 |
| (+-)-Fenfluramine hydrochloride | N-Ethyl-alpha-methyl-3-(trifluoromethyl)benzeneethanamine hydrochloride (+-)- | Fenfluramine H |
| Racemic fenfluramine hydrochloride | Benzeneethanamine, N-ethyl-alpha-methyl-3-(trifluoromethyl)-, hydrochloride, (+-)- | CHEMBL21062 |
| Fenfluramine hydrochloride [USAN] | Fenfluramine hydrochloride (USAN) | DTXSID309364 |

PubChem

# 3 Chemical and Physical Properties

## 3.1 Computed Properties

| Property Name | Property Value | Reference |
|---|---|---|
| Molecular Weight | 267.72 g/mol | Computed by PubChem 2.1 (PubChem release 2019.06.18) |
| Hydrogen Bond Donor Count | 2 | Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) |
| Hydrogen Bond Acceptor Count | 4 | Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) |
| Rotatable Bond Count | 4 | Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) |
| Exact Mass | 267.100162 g/mol | Computed by PubChem 2.1 (PubChem release 2019.06.18) |
| Monoisotopic Mass | 267.100162 g/mol | Computed by PubChem 2.1 (PubChem release 2019.06.18) |
| Topological Polar Surface Area | 12 Å² | Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) |
| Heavy Atom Count | 17 | Computed by PubChem |
| Formal Charge | 0 | Computed by PubChem |
| Complexity | 203 | Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18) |
| Isotope Atom Count | 0 | Computed by PubChem |
| Defined Atom Stereocenter Count | 0 | Computed by PubChem |
| Undefined Atom Stereocenter Count | 1 | Computed by PubChem |
| Defined Bond Stereocenter Count | 0 | Computed by PubChem |
| Undefined Bond Stereocenter Count | 0 | Computed by PubChem |
| Covalently-Bonded Unit Count | 2 | Computed by PubChem |
| Compound Is Canonicalized | Yes | Computed by PubChem (release 2019.01.04) |

PubChem

# 4 Spectral Information

## 4.1 IR Spectra

### 4.1.1 ATR-IR Spectra

| | |
|---|---|
| Instrument Name | Bio-Rad FTS |
| Technique | ATR-Neat (DuraSamplIR II) |
| Source of Spectrum | Forensic Spectral Research |
| Source of Sample | Alltech Associates, Inc., Grace Davison Discovery Sciences |
| Catalog Number | 01798 |
| Lot Number | 27082 |
| Copyright | Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved. |
| Thumbnail | |

SpectraBase

## 4.2 Raman Spectra

| | |
|---|---|
| Technique | FT-Raman |
| Source of Spectrum | Forensic Spectral Research |
| Source of Sample | Alltech Associates, Inc., Grace Davison Discovery Sciences |
| Catalog Number | 01798 |
| Lot Number | 27082 |
| Copyright | Copyright © 2012-2018 Bio-Rad Laboratories, Inc. All Rights Reserved. |
| Thumbnail | |

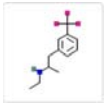
SpectraBase

# 5 Related Records

## 5.1 Related Compounds with Annotation

PubChem

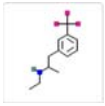
## 5.2 Parent Compound



CID 3337 (Fenfluramine)

PubChem

## 5.3 Component Compounds



CID 3337 (Fenfluramine)



CID 313 (Hydrochloric acid)

PubChem

## 5.4 Related Compounds

| | |
|---|---|
| Same Connectivity | 4 Records |
| Same Stereo | 2 Records |
| Same Isotope | 3 Records |

| | |
|---|---|
| Same Parent, Connectivity | 62 Records |
| Same Parent, Stereo | 49 Records |
| Same Parent, Isotope | 58 Records |
| Same Parent, Exact | 45 Records |
| Mixtures, Components, and Neutralized Forms | 2 Records |
| Similar Compounds | 543 Records |

PubChem

## 5.5 Substances

### 5.5.1 Related Substances

| | |
|---|---|
| Same | 47 Records |

PubChem

### 5.5.2 Substances by Category

PubChem

## 5.6 Entrez Crosslinks

| | |
|---|---|
| Gene | 4 Records |

PubChem

## 5.7 NCBI LinkOut

NCBI

## 6 Chemical Vendors

PubChem

# 7 Drug and Medication Information

## 7.1 Drug Indication

Adjunctive therapy to diet, in patients with obesity and a body mass index (BMI) of 30 kg/m2 or higher who have not responded to an appropriate weight-reducing regimen alone

- EU Community Register of Medicinal Products

Treatment of Dravet syndrome

- EU Community Register of Medicinal Products

Treatment of Lennox-Gastaut syndrome

- EU Community Register of Medicinal Products

## 7.2 Clinical Trials

### 7.2.1 ClinicalTrials.gov

- ClinicalTrials.gov

### 7.2.2 EU Clinical Trials Register

EU Clinical Trials Register

### 7.2.3 NIPH Clinical Trials Search of Japan

NIPH Clinical Trials Search of Japan

## 7.3 EMA Drug Information

| | |
|---|---|
| Medicine | Enpaxiq |
| Disease/Condition | Treatment of Dravet syndrome |
| Active Substance | Fenfluramine hydrochloride |
| Status of Orphan Designation | Positive |
| Decision Date | 2014-01-16 |

European Medicines Agency (EMA)

# 8 Pharmacology and Biochemistry

## 8.1 Pharmacology

Fenfluramine Hydrochloride is the hydrochloride salt of fenfluramine, an amphetamine derivative and a sympathomimetic stimulant with appetite-suppressant properties. Fenfluramine, which was part of the Fen-Phen anti-obesity medication, stimulates the release of serotonin from vesicular storage, and modulates serotonin transporter function. Since serotonin regulates mood and appetite, among other functions, increased serotonin level results in a feeling of fullness and loss of appetite.

- NCI Thesaurus (NCIt)

## 8.2 MeSH Pharmacological Classification

Serotonin Agents

Drugs used for their effects on serotonergic systems. Among these are drugs that affect serotonin receptors, the life cycle of serotonin, and the survival of serotonergic neurons. (See all compounds classified as Serotonin Agents.)

- MeSH

Serotonin Uptake Inhibitors

Compounds that specifically inhibit the reuptake of serotonin in the brain. (See all compounds classified as Serotonin Uptake Inhibitors.)

- MeSH

# 9 Use and Manufacturing

## 9.1 Use Classification

| | |
|---|---|
| EU Pharmaceutical Product Classes | Human drug |

▶ EU Community Register of Medicinal Products

| | |
|---|---|
| EU Pharmaceutical Product Classes | Human drug |

▶ EU Community Register of Medicinal Products

| | |
|---|---|
| EU Pharmaceutical Product Classes | Human drug |

▶ EU Community Register of Medicinal Products

| | |
|---|---|
| Drug Active Substance | Fenfluramine hydrochloride |
| EMA Drug Category | Human, Rare disease (orphan) |

▶ European Medicines Agency (EMA)

# 10 Safety and Hazards

## 10.1 Hazards Identification

### 10.1.1 GHS Classification

Showing 1 of 2 View More

| | |
|---|---|
| Pictogram(s) |  Acute Toxic  Irritant |
| Signal | Danger |
| GHS Hazard Statements | Aggregated GHS information provided by 2 companies from 2 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.<br>H300 (50%): Fatal if swallowed [Danger Acute toxicity, oral]<br>H302 (50%): Harmful if swallowed [Warning Acute toxicity, oral]<br>Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown. |
| Precautionary Statement Codes | P264, P270, P301+P310, P301+P312, P321, P330, P405, and P501<br>(The corresponding statement to each P-code can be found at the GHS Classification page.) |

▸ European Chemicals Agency (ECHA)

# 11 Toxicity

## 11.1 Toxicological Information

### 11.1.1 Acute Effects

- ChemIDplus

# 12 Literature

## 12.1 NLM Curated PubMed Citations

PubChem

## 12.2 Springer Nature References

Springer Nature

## 12.3 Chemical Co-Occurrences in Literature

PubChem

## 12.4 Chemical-Gene Co-Occurrences in Literature

PubChem

## 12.5 Chemical-Disease Co-Occurrences in Literature

PubChem

# 13 Patents

## 13.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

## 13.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=ZXKXJHAOUFHNAS-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

# 14 Biological Test Results

## 14.1 BioAssay Results

PubChem

# 15 Classification

## 15.1 Ontologies

### 15.1.1 MeSH Tree

▶ MeSH

### 15.1.2 KEGG: ATC

▶ KEGG

### 15.1.3 KEGG: Target-based Classification of Drugs

KEGG

### 15.1.4 KEGG: Drug Classes

KEGG

### 15.1.5 WHO ATC Classification System

▶ WHO ATC

## 15.1.6 WIPO IPC

▶ WIPO

## 15.1.7 ChemIDplus

- ChemIDplus

## 15.1.8 UN GHS Classification

- UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

# 16 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ## ChemIDplus

*Fenfluramine hydrochloride [USAN]*
*https://chem.nlm.nih.gov/chemidplus/sid/0000404820*

*ChemIDplus Chemical Information Classification*
*https://chem.sis.nlm.nih.gov/chemidplus/*

2. ## European Chemicals Agency (ECHA)

> LICENSE
>
> Use of the information, documents and data from the ECHA website is subject to the terms and conditions of this Legal Notice, and subject to other binding limitations provided for under applicable law, the information, documents and data made available on the ECHA website may be reproduced, distributed and/or used, totally or in part, for non-commercial purposes provided that ECHA is acknowledged as the source: "Source: European Chemicals Agency, http://echa.europa.eu/". Such acknowledgement must be included in each copy of the material. ECHA permits and encourages organisations and individuals to create links to the ECHA website under the following cumulative conditions: Links can only be made to webpages that provide a link to the Legal Notice page.
>
> https://echa.europa.eu/web/guest/legal-notice

*fenfluramine hydrochloride*
*https://echa.europa.eu/substance-information/-/substanceinfo/100.006.336*

*Fenfluramine hydrochloride*
*https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/31889*

*(±)-N-Ethyl-α-methyl-m-[trifluoromethyl]phenethylaminehydrochloride*
*https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/157116*

3. ## ClinicalTrials.gov

> LICENSE
>
> The ClinicalTrials.gov data carry an international copyright outside the United States and its Territories or Possessions. Some ClinicalTrials.gov data may be subject to the copyright of third parties; you should consult these entities for any additional terms of use.
>
> https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

*https://clinicaltrials.gov/*

4. ## EU Clinical Trials Register

*https://www.clinicaltrialsregister.eu/*

5. ## EU Community Register of Medicinal Products

*Fenfluramine*
*https://ec.europa.eu/health/documents/community-register/html/ho1044.htm*

*Fenfluramine hydrochloride*
*https://ec.europa.eu/health/documents/community-register/html/o1219.htm*

*Fenfluramine hydrochloride*
*https://ec.europa.eu/health/documents/community-register/html/o1836.htm*

6. ## European Medicines Agency (EMA)

*Fenfluramine hydrochloride(EU/3/14/1219)*
*https://www.ema.europa.eu/en/medicines/human/orphan-designations/eu3141219*

7. NCI Thesaurus (NCIt)



*Fenfluramine Hydrochloride*
*https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C75112*

8. NIPH Clinical Trials Search of Japan
*https://rctportal.niph.go.jp/en/*

9. SpectraBase
*https://spectrabase.com/spectrum/1be55QN7L2W*
*https://spectrabase.com/spectrum/CPmVyiplYG0*

10. Springer Nature
*https://pubchem.ncbi.nlm.nih.gov/substance/341188590*
*https://pubchem.ncbi.nlm.nih.gov/substance/341197047*

11. Wikipedia
*fenfluramine hydrochloride*
*https://www.wikidata.org/wiki/Q27126872*

12. MeSH
*Fenfluramine*
*https://www.ncbi.nlm.nih.gov/mesh/68005277*
*MeSH Tree*
*http://www.nlm.nih.gov/mesh/meshhome.html*
*Serotonin Agents*
*https://www.ncbi.nlm.nih.gov/mesh/68018490*
*Serotonin Uptake Inhibitors*
*https://www.ncbi.nlm.nih.gov/mesh/68017367*

13. PubChem
*https://pubchem.ncbi.nlm.nih.gov*

14. KEGG
*Anatomical Therapeutic Chemical (ATC) classification*
*http://www.genome.jp/kegg-bin/get_htext?br08303.keg*
*Target-based classification of drugs*
*http://www.genome.jp/kegg-bin/get_htext?br08310.keg*
*Drug Classes*
*http://www.genome.jp/kegg-bin/get_htext?br08330.keg*

15. WIPO
*International Patent Classification*
*http://www.wipo.int/classifications/ipc/*

16. WHO ATC
*ATC Code*
*https://www.whocc.no/atc_ddd_index/*

17. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)
*GHS Classification Tree*
*http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html*

18. PATENTSCOPE (WIPO)
    *SID 388352874*
    *https://pubchem.ncbi.nlm.nih.gov/substance/388352874*

19. NCBI
    *https://www.ncbi.nlm.nih.gov/projects/linkout*