

Fexofenadine
hydrochloride
C32H40ClNO4
structure



**ASSIGN
BUSTER**

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- Bio Activity:

Molecular C₃₂ H₄₀ ClNO

Formula 4

Average mass 538. 117 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:**

148-150 °CLKT

Labs[F1895]

190-192

°CLabNetworkLN001767

69

- **Experimental Boiling Point:**

697.3 °CLKT

Labs[F1895]

- **Experimental Solubility:**

50 mM in

DMSOMedChem

Expresshttp://www.

medchemexpress.

com/Terbutaline-sulfate.

html

DMSO to 50 mM, water

to 2 mg/mL, ethanol to

107 mg/mL,

methanolLKT

Labs[F1895]

DMSO:

50mg/mLMedChem

ExpressHY-B0801A

Soluble in DMSOAxon

Medchem1453

Soluble to 50 mM in

DMSOTocris

Bioscience2429

- Miscellaneous

- **Safety:**

5Axon Medchem1453

H303; H313; H317;

H333; H334; H335;

H373Axon

Medchem1453

IRRITANTMatrix

Scientific076066

no pictogramAxon

Medchem1453

NoneLKT Labs[F1895]

P101; P102; P103; P260;

P262; P263; P264; P270;

P280; P304; P312;

P340Axon Medchem1453

WarningAxon

Medchem1453

- **Target Organs:**

Histamine Receptor

antagonistTargetMolT147

0, T1470L

- **Drug Status:**

approvedBIONET-Key

OrganicsKS-1057

- **Compound Source:**

syntheticMicrosource[0150

4179]

- **Bio Activity:**

7-TM ReceptorsTocris

Bioscience2429

Fexofenadine is a third-generation antihistamine pharmaceutical drug used in the treatment of allergy symptoms, such as hay fever, nasal congestion, and urticaria.

MedChem

Express[http://www.](http://www.medchemexpress.com/Terbutaline-sulfate)

medchemexpress.

com/Terbutaline-sulfate.

html, HY-B0801A

GPCR/G proteinMedChem

ExpressHY-B0801A

GPCR/G protein;

MedChem ExpressHY-

B0801A

H1 receptor antagonist;

non-sedating antiallergic

agentTocris

Bioscience2429

Histamine H1

receptorTargetMolT1470,

T1470L

Histamine H1

ReceptorsTocris

Bioscience2429

Histamine

ReceptorMedChem

ExpressHY-B0801A

Histamine

ReceptorsTocris

Bioscience2429

NeuroscienceTargetMolT

1470, T1470L

Selective histamine H1
receptor antagonist (pKi
= 8. 1). Active
metabolite of terfenadine
that displays non-
sedating antiallergic
effects. Tocris
Bioscience2429

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

No predicted properties have been calculated for this compound.

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