

# [Fexofenadine hydrochloride c32h40clno4 structure](https://assignbuster.com/fexofenadine-hydrochloride-c32h40clno4-structure/)

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* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula | C 32 H 40 ClNO 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 °CLabNetworkLN00176769 |

## 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 antagonistTargetMolT1470, T1470L |

## Drug Status:

|  |
| --- |
| approvedBIONET-Key OrganicsKS-1057 |

## Compound Source:

|  |
| --- |
| syntheticMicrosource[01504179] |

## 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 Expresshttp://www. 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 |
| NeuroscienceTargetMolT1470, 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