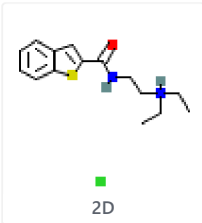
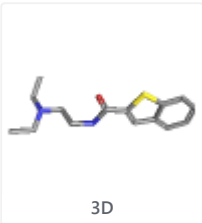
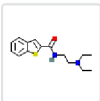



## COMPOUND SUMMARY

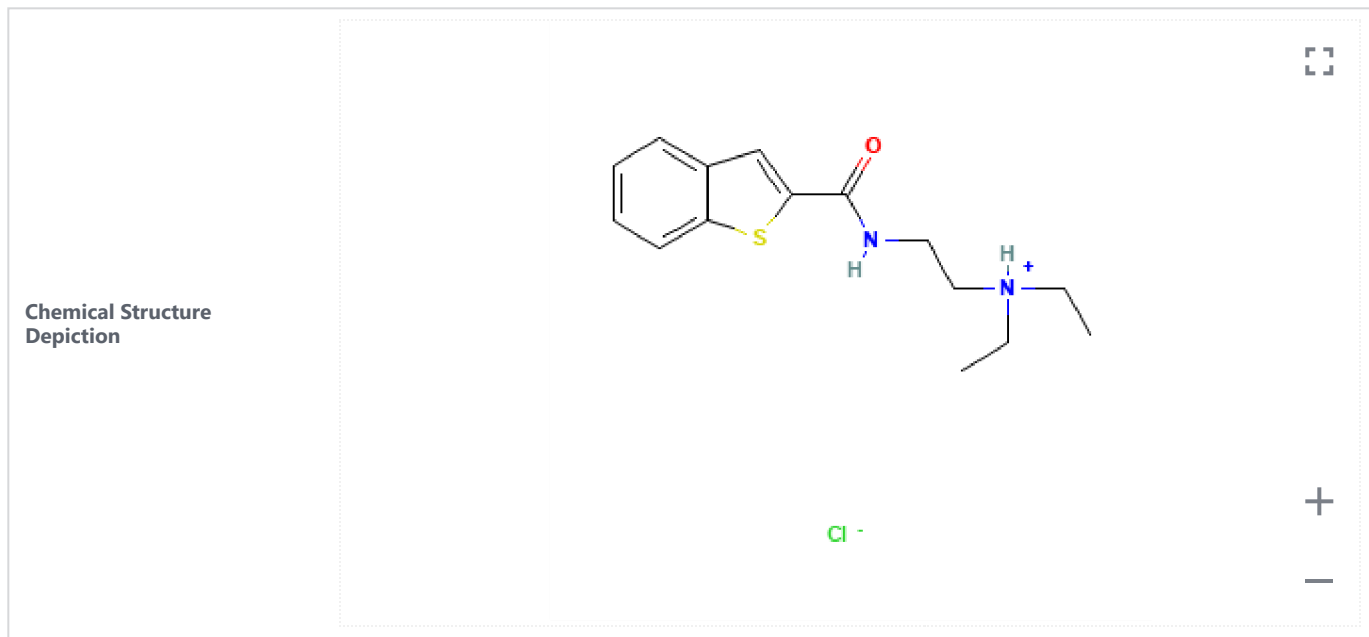
# Macrolog 4000

<b>PubChem CID</b>	27174				
<b>Structure</b>	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>2D</p> </div> <div style="text-align: center;">  <p>3D</p> </div> </div> <p style="text-align: center;"><a href="#">Find Similar Structures</a></p>				
<b>Molecular Formula</b>	C <sub>15</sub> H <sub>21</sub> CIN <sub>2</sub> OS				
<b>Synonyms</b>	<p>Macrolog 4000          UNII-FZ46ONU496          FZ46ONU496          NSC 108963          Macrolog 4000 [INN]</p> <p><a href="#">More...</a></p>				
<b>Molecular Weight</b>	312.9				
<b>Parent Compound</b>	 <p><a href="#">CID 27175 (Benzo(b)thiophene-2-carboxamide, N-(2-(diethylamino)ethyl)-)</a></p>				
<b>Component Compounds</b>	 <p><a href="#">CID 313 (Hydrochloric acid)</a></p>  <p><a href="#">CID 27175 (Benzo(b)thiophene-2-carboxamide, N-(2-(diethylamino)ethyl)-)</a></p>				
<b>Dates</b>	<table style="width: 100%;"> <tr> <td style="width: 50%;">Modify</td> <td style="width: 50%;">Create</td> </tr> <tr> <td>2022-05-28</td> <td>2005-08-08</td> </tr> </table>	Modify	Create	2022-05-28	2005-08-08
Modify	Create				
2022-05-28	2005-08-08				

# 1 Structures



## 1.1 2D Structure

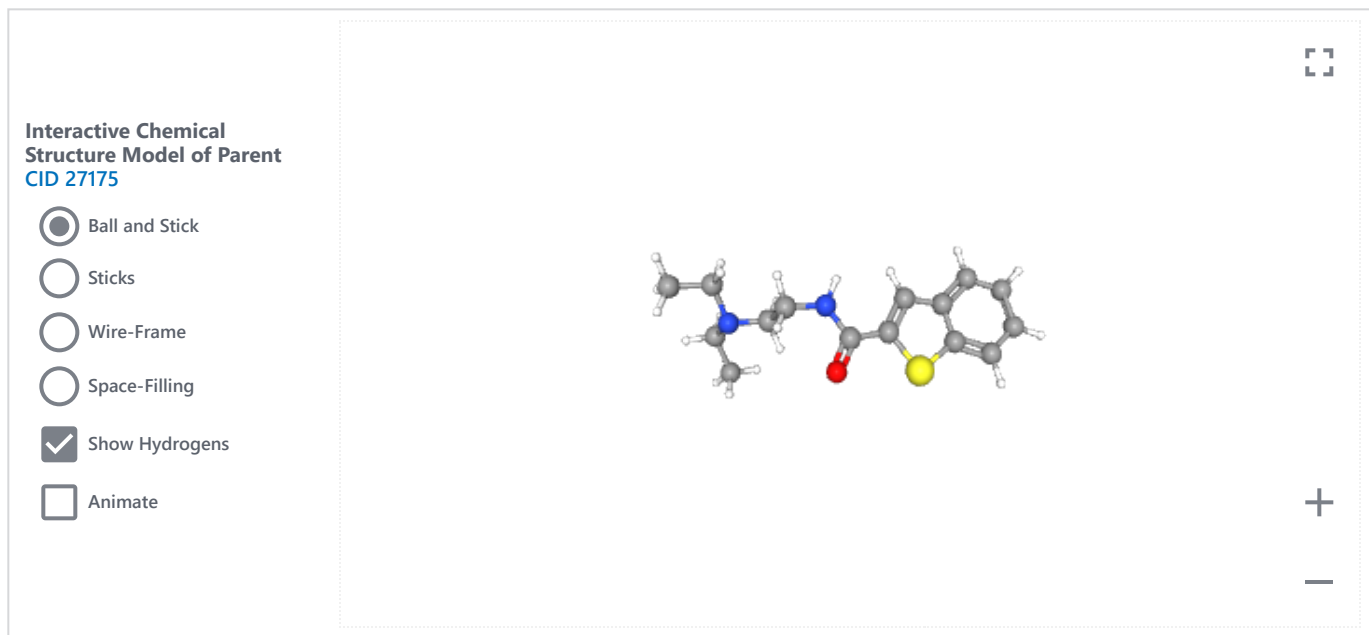


► PubChem

## 1.2 3D Conformer



### 3D Conformer of Parent



► PubChem

## 2 Names and Identifiers

### 2.1 Computed Descriptors

#### 2.1.1 IUPAC Name

2-(1-benzothiophene-2-carbonylamino)ethyl-diethylazanium;chloride

*Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)*

[▶ PubChem](#)

#### 2.1.2 InChI

InChI=1S/C15H20N2OS.ClH/c1-3-17(4-2)10-9-16-15(18)14-11-12-7-5-6-8-13(12)19-14;/h5-8,11H,3-4,9-10H2,1-2H3,(H,16,18);1H

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

[▶ PubChem](#)

#### 2.1.3 InChI Key

TZBAVQKIEKDGFB-UHFFFAOYSA-N

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

[▶ PubChem](#)

#### 2.1.4 Canonical SMILES

CC[NH+](CC)CCNC(=O)C1=CC2=CC=CC=C2S1.[Cl-]

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

[▶ PubChem](#)

## 2.2 Molecular Formula

C15H21CIN2OS

*Computed by PubChem 2.1 (PubChem release 2021.05.07)*

[▶ PubChem](#)

## 2.3 Other Identifiers

### 2.3.1 CAS

15272-95-4

[▶ ChemIDplus](#)

## 2.4 Synonyms



## 2.4.1 Depositor-Supplied Synonyms

Macrogol 4000

UNII-FZ46ONU496

FZ46ONU496

NSC 108963

Macrogol 4000 [INN]

Macrogol4000

**BENZO(b)THIOPHENE-2-CARBOXAMIDE, N-(2-(DIETHYLAMINO)ETHYL)-, HYDROCHLORIDE**

Benzo(b)thiophene-2-carboxamide, N-(2-(diethylamino)ethyl)-, monohydrochloride

▶ [PubChem](#)

## 3 Chemical and Physical Properties



### 3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	312.9	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	312.1063122	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	312.1063122	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	61.8 Å <sup>2</sup>	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	20	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	294	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	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 2021.05.07)

► [PubChem](#)

## 4 Related Records

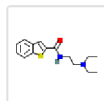


### 4.1 Related Compounds with Annotation



▶ PubChem

### 4.2 Parent Compound



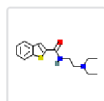
CID 27175 (Benzo(b)thiophene-2-carboxamide, N-(2-(diethylamino)ethyl)-)

▶ PubChem

### 4.3 Component Compounds



CID 313 (Hydrochloric acid)



CID 27175 (Benzo(b)thiophene-2-carboxamide, N-(2-(diethylamino)ethyl)-)

▶ PubChem

### 4.4 Related Compounds



Same Parent, Exact	3 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	787 Records

▶ PubChem

## 4.5 Substances



### 4.5.1 Related Substances



Same	10 Records
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▶ PubChem

### 4.5.2 Substances by Category



▶ PubChem

## 5 Drug and Medication Information



### 5.1 Drug Indication



Bowel cleansing prior to clinical procedures

▶ [European Medicines Agency \(EMA\)](#)

### 5.2 Clinical Trials



#### 5.2.1 ClinicalTrials.gov



▶ [ClinicalTrials.gov](#)

#### 5.2.2 EU Clinical Trials Register



▶ [EU Clinical Trials Register](#)



### 5.2.3 NIPH Clinical Trials Search of Japan



▶ [NIPH Clinical Trials Search of Japan](#)

### 5.3 EMA Drug Information



<b>Active Substance</b>	<a href="#">citric acid</a> (as <a href="#">citric acid anhydrous</a> ), <a href="#">macrogol 4000</a> , <a href="#">potassium chloride</a> , <a href="#">simeticone</a> , <a href="#">sodium chloride</a> , <a href="#">sodium citrate</a> , <a href="#">sodium sulfate</a> (as <a href="#">sodium sulfate anhydrous</a> )
<b>Therapeutic Area</b>	Gastroentology-Hepatology
<b>Drug Form</b>	Powder for oral suspension
<b>Administration Route</b>	Oral use
<b>Decision Type</b>	PM: decision on the application for modification of an agreed PIP
<b>Decision Date</b>	2021-04-14

▶ [European Medicines Agency \(EMA\)](#)

## 6 Use and Manufacturing



### 6.1 Uses



#### 6.1.1 Use Classification



Human Drugs -> EU pediatric investigation plans

- ▶ [European Medicines Agency \(EMA\)](#)

## 7 Toxicity



### 7.1 Toxicological Information



#### 7.1.1 Acute Effects



► [ChemIDplus](#)

## 8 Literature



### 8.1 Springer Nature References



▶ Springer Nature

### 8.2 Chemical Co-Occurrences in Literature



▶ PubChem

### 8.3 Chemical-Gene Co-Occurrences in Literature



▶ PubChem

## 8.4 Chemical-Disease Co-Occurrences in Literature

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▶ PubChem

## 9 Patents



### 9.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

### 9.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

▶ PATENTSCOPE (WIPO)

## 10 Classification



### 10.1 Ontologies



#### 10.1.1 ChemIDplus



► ChemIDplus

# 11 Information Sources



FILTER BY SOURCE

ALL SOURCES



## 1. ChemIDplus

### LICENSE

<https://www.nlm.nih.gov/copyright.html>

Macrogol 4000 [INN]

<https://chem.nlm.nih.gov/chemidplus/sid/0015272954>

ChemIDplus Chemical Information Classification

<https://chem.nlm.nih.gov/chemidplus/>

## 2. ClinicalTrials.gov

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<https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use>

<https://clinicaltrials.gov/>

## 3. EU Clinical Trials Register

<https://www.clinicaltrialsregister.eu/>

## 4. European Medicines Agency (EMA)

### LICENSE

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<https://www.ema.europa.eu/en/about-us/legal-notice>

*citric acid (as citric acid anhydrous), macrogol 4000, potassium chloride, simeticone, sodium chloride, sodium citrate, sodium sulfate (as sodium sulfate anhydrous) (P/0134/2021)*

<https://www.ema.europa.eu/en/medicines/human/paediatric-investigation-plans/emea-001356-pip02-12-m04>

## 5. NIPH Clinical Trials Search of Japan

<https://rctportal.niph.go.jp/en/>

## 6. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/341199096>

## 7. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

## 8. PATENTSCOPE (WIPO)

SID 388872140

<https://pubchem.ncbi.nlm.nih.gov/substance/388872140>