

## COMPOUND SUMMARY

# 2-Amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride



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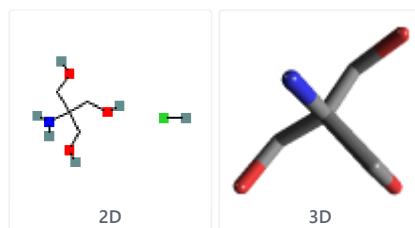
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PubChem CID: 93573

Structure:


[Find Similar Structures](#)

Chemical Safety:



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)
Molecular Formula:  $C_4H_{12}ClNO_3$ 

Chemical Names:

1185-53-1  
 Tris hydrochloride  
 Tris(hydroxymethyl)aminomethane hydrochloride  
 2-Amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride  
 Tromethamine hydrochloride

[More...](#)

Molecular Weight: 157.59 g/mol

Dates:

Modify: 2019-08-10  
 Create: 2005-08-08

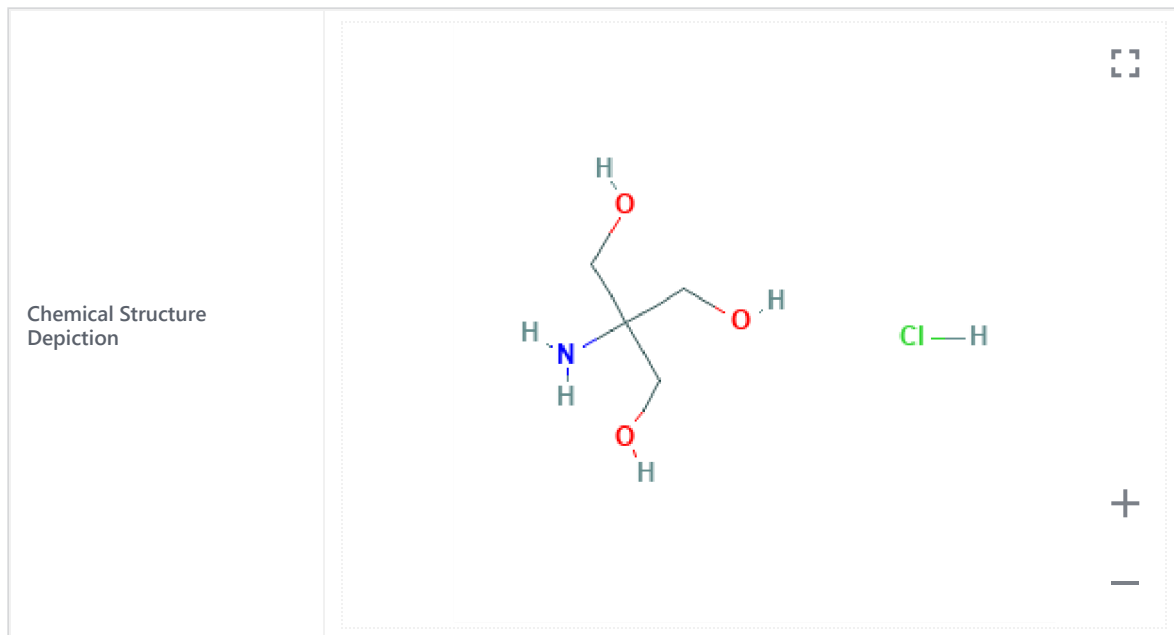
# 1 Structures



## 1.1 2D Structure



Find Similar Structures Get Image Download



▶ from PubChem

## 1.2 3D Conformer



3D Conformer of Parent

▶ from PubChem

## 2 Names and Identifiers

### 2.1 Computed Descriptors

#### 2.1.1 IUPAC Name

2-amino-2-(hydroxymethyl)propane-1,3-diol;hydrochloride

▶ from PubChem

#### 2.1.2 InChI

InChI=1S/C4H11NO3.ClH/c5-4(1-6,2-7)3-8;/h6-8H,1-3,5H2;1H

▶ from PubChem

#### 2.1.3 InChI Key

QKNYBSVHEMOAJP-UHFFFAOYSA-N

▶ from PubChem

#### 2.1.4 Canonical SMILES

C(C(CO)(CO)N)O.Cl

▶ from PubChem

## 2.2 Molecular Formula



C<sub>4</sub>H<sub>12</sub>ClNO<sub>3</sub>

▶ from PubChem

## 2.3 Other Identifiers



### 2.3.1 CAS



1185-53-1

▶ from ChemIDplus; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

#### Other CAS

35087-75-3

150551-82-9

▶ from ChemIDplus

### 2.3.2 European Community (EC) Number



214-684-5

▶ from European Chemicals Agency (ECHA)

### 2.3.3 UNII



383V75M34E

▶ from FDA/SPL Indexing Data

### 2.3.4 Wikipedia



Tromethamine hydrochloride

▶ from Wikipedia

## 2.4 Synonyms



### 2.4.1 Depositor-Supplied Synonyms



1185-53-1	383V75M34E
Tris hydrochloride	AK-41164
Tris(hydroxymethyl)aminomethane hydrochloride	Trometamol, Tromethamine, Tris-[hydroxymethyl]aminom
2-Amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride	Trometamol, Tromethamine, Tris-[hydroxymethyl]aminom
Tromethamine hydrochloride	Tris chloride
TRIS HCl	Tromethamine HCl
2-Amino-2-(hydroxymethyl)-1,3-propanediol Hydrochloride	Trizma hydrochloride
Tris-HCl	Tris hydrochloride buffer
MFCD00012590	Tris(hydroxymethyl)aminomethane hydrochloride, 99+%,
UNII-383V75M34E	TrisHCl
Trizma(R) hydrochloride	Tris.HCl
1,3-Propanediol, 2-amino-2-(hydroxymethyl)-, hydrochloride	EINECS 214-684-5
2-Amino-2-hydroxymethyl-1,3-propanediol hydrochloride	Tris (hydrochloride)

▶ from PubChem

## 3 Chemical and Physical Properties



### 3.1 Computed Properties



Property Name	Property Value
Molecular Weight	157.59 g/mol
Hydrogen Bond Donor Count	5
Hydrogen Bond Acceptor Count	4
Rotatable Bond Count	3
Exact Mass	157.050571 g/mol
Monoisotopic Mass	157.050571 g/mol
Topological Polar Surface Area	86.7 A <sup>2</sup>
Heavy Atom Count	9
Formal Charge	0

Property Name	Property Value
Complexity	54
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	2
Compound Is Canonicalized	Yes

▶ from PubChem

## 4 Spectral Information



### 4.1 1D NMR Spectra



#### 4.1.1 1H NMR Spectra



Instrument Name	Varian A-60
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

## 4.1.2 <sup>13</sup>C NMR Spectra



Source of Sample	Eastman Organic Chemicals, Rochester, New York
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

## 4.2 IR Spectra



### 4.2.1 FTIR Spectra



Technique	KBr WAFER
Source of Sample	EASTMAN ORGANIC CHEMICALS, ROCHESTER, NEW YORK
Catalog Number	11511
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	



▶ from SpectraBase

#### 4.2.2 ATR-IR Spectra



Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat (DuraSAMPLIR II)
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Spectrochem Pvt. Ltd.
Catalog Number	42062
Copyright	Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	





▶ from SpectraBase

## 4.3 Raman Spectra



Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories
Source of Sample	Spectrochem Pvt. Ltd., India
Catalog Number	42062
Copyright	Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

## 5 Related Records



## 5.1 Related Compounds with Annotation



▶ from PubChem

## 5.2 Parent Compound



6503

▶ from PubChem

## 5.3 Related Compounds



Same Parent, Connectivity	98 Records
Same Parent, Exact	93 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	29 Records

▶ from PubChem

## 5.4 Substances



### 5.4.1 Related Substances



Same

139 Records

▶ from PubChem

### 5.4.2 Substances by Category



▶ from PubChem

## 6 Chemical Vendors



▶ from PubChem

## 7 Use and Manufacturing

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### 7.1 Uses

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EPA CPDat Chemical and Product Categories

▶ from EPA Chemical and Products Database (CPDat)

#### 7.1.1 Industry Uses

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Laboratory chemicals

<https://www.epa.gov/chemical-data-reporting>

▶ from EPA Chemicals under the TSCA

## 7.2 General Manufacturing Information



### Industry Processing Sectors

Wholesale and retail trade

▶ from EPA Chemicals under the TSCA

### EPA TSCA Commercial Activity Status

**1,3-Propanediol, 2-amino-2-(hydroxymethyl)-, hydrochloride (1:1): ACTIVE**

<https://www.epa.gov/tsca-inventory>

▶ from EPA Chemicals under the TSCA

## 8 Safety and Hazards




### 8.1 Hazards Identification



#### 8.1.1 GHS Classification



Pictogram(s)	 Irritant
Signal	<b>Warning</b>
GHS Hazard Statements	<p>Aggregated GHS information provided by 172 companies from 15 notifications to the ECHA C&amp;L Inventory. Each notification may be associated with multiple companies.</p> <p>Reported as not meeting GHS hazard criteria by 74 of 172 companies. For more detailed information, please visit <a href="#">ECHA C&amp;L website</a></p> <p>Of the 13 notification(s) provided by 98 of 172 companies with hazard statement code(s):</p> <p>H315 (100%): Causes skin irritation [<b>Warning</b> Skin corrosion/irritation]</p> <p>H319 (100%): Causes serious eye irritation [<b>Warning</b> Serious eye damage/eye irritation]</p>

	<p>H335 (95.92%): May cause respiratory irritation [<a href="#">Warning</a> Specific target organ toxicity, single exposure; Respiratory tract irritation]</p> <p>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.</p>
Precautionary Statement Codes	<p>P261, P264, P271, P280, P302+P352, P304+P340, P305+P351+P338, P312, P321, P332+P313, P337+P313, P362, P403+P233, P405, and P501</p> <p>(The corresponding statement to each P-code can be found at the <a href="#">GHS Classification</a> page.)</p>

▶ from European Chemicals Agency (ECHA)

## 9 Literature



### 9.1 Springer Nature References



▶ from Springer Nature

### 9.2 Chemical Co-Occurrences in Literature



▶ from PubChem

## 9.3 Chemical-Disease Co-Occurrences in Literature

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▶ from PubChem

## 9.4 Chemical-Gene Co-Occurrences in Literature

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▶ from PubChem

## 10 Patents

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### 10.1 Depositor-Supplied Patent Identifiers

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▶ from PubChem

## 11 Biological Test Results



### 11.1 BioAssay Results



▶ from PubChem

## 12 Classification



### 12.1 Ontologies



#### 12.1.1 WHO ATC Classification System



▶ from WHO ATC

### 12.1.2 WIPO IPC

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▶ from WIPO

### 12.1.3 ChemIDplus

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▶ from ChemIDplus

#### 12.1.4 UN GHS Classification

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

#### 12.1.5 EPA CPDat Classification

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▶ from EPA Chemical and Products Database (CPDat)

## 13 Information Sources



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ALL SOURCES



### 1. ChemIDplus

*Tromethamine hydrochloride*

<https://chem.nlm.nih.gov/chemidplus/sid/0001185531>

*ChemIDplus Chemical Information Classification*

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

### 2. EPA Chemicals under the TSCA

#### LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

*1,3-Propanediol, 2-amino-2-(hydroxymethyl)-, hydrochloride (1:1)*

<https://www.epa.gov/chemicals-under-tsca>

### 3. EPA DSSTox

*Tromethamine hydrochloride*

<https://comptox.epa.gov/dashboard/DTXSID4044373>

### 4. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

*2-amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride*

<https://echa.europa.eu/substance-information/-/substanceinfo/100.013.349>

*2-amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride*

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/26910>

**5. EPA Chemical and Products Database (CPDat)****LICENSE**

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

*2-amino-2-(hydroxymethyl)propane-1,3-diol hydrochloride*

<https://comptox.epa.gov/dashboard/DTXSID4044373#exposure>

*EPA CPDat Classification*

<https://www.epa.gov/chemical-research/chemical-and-products-database-cpd>

**6. FDA/SPL Indexing Data**

*383V75M34E*

<https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/>

**7. SpectraBase**

<https://spectrabase.com/spectrum/CiZJPOpXvbM>

<https://spectrabase.com/spectrum/Ak71GZLlpGH>

<https://spectrabase.com/spectrum/DRWyD3xmPvD>

<https://spectrabase.com/spectrum/6sQyLxr57CF>

<https://spectrabase.com/spectrum/LF0U7FCLx8o>

**8. Springer Nature****9. Wikipedia**

*tromethamine hydrochloride*

<https://www.wikidata.org/wiki/Q27256734>

**10. PubChem**

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

**11. WIPO**

*International Patent Classification*

<http://www.wipo.int/classifications/ipc/>

**12. WHO ATC**

*ATC Code*

[https://www.whocc.no/atc\\_ddd\\_index/](https://www.whocc.no/atc_ddd_index/)

13. **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](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)