

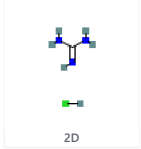


## COMPOUND SUMMARY

## Guanidine hydrochloride

[Cite](#) [Download](#)

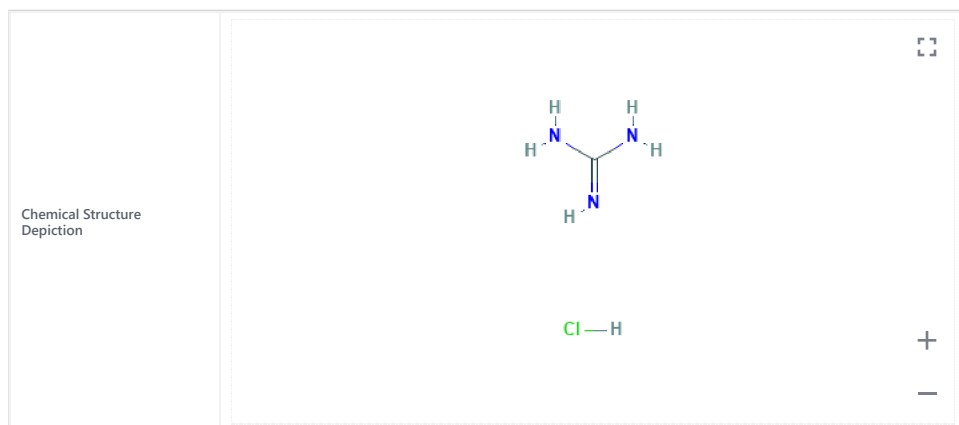
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PubChem CID:	5742
Structure:	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>2D</p> </div> <div style="text-align: center;">  <p>3D</p> </div> </div> <p><a href="#">Find Similar Structures</a></p>
Chemical Safety:	<div style="text-align: center;">  <p>Irritant</p> <p><a href="#">Laboratory Chemical Safety Summary (LCSS) Datasheet</a></p> </div>
Molecular Formula:	CH <sub>5</sub> ClN <sub>3</sub> or CH <sub>5</sub> N <sub>3</sub> .ClH
Chemical Names:	Guanidine hydrochloride 50-01-1 Guanidinium chloride guanidine HCl Guanidine, monohydrochloride <input type="button" value="More..."/>
Molecular Weight:	95.53 g/mol
Dates:	Modify: 2019-08-03    Create: 2005-07-19
<p>Guanidine Hydrochloride is the hydrochloride salt form of <a href="#">guanidine</a>, a strong basic compound with parasymphomimetic activity. Guanidine hydrochloride enhances the release of <a href="#">acetylcholine</a> following a nerve impulse and potentiates <a href="#">acetylcholine</a> actions on muscarinic and nicotinic receptors. It also appears to slow the rates of depolarization and repolarization of muscle cell membranes. (NCI05)</p> <p><a href="#">from NCI</a></p> <p>A strong organic base existing primarily as guanidium ions at physiological pH. It is found in the urine as a normal product of protein metabolism. It is also used in laboratory research as a protein denaturant. (From Martindale, the Extra Pharmacopoeia, 30th ed and Merck Index, 12th ed) It is also used in the treatment of myasthenia and as a fluorescent probe in HPLC.</p> <p><a href="#">from MeSH</a></p>	

1 Structures ?[↗](#)1.1 2D Structure ?[↗](#)

[Find Similar Structures](#) [Get Image](#) [Download](#)



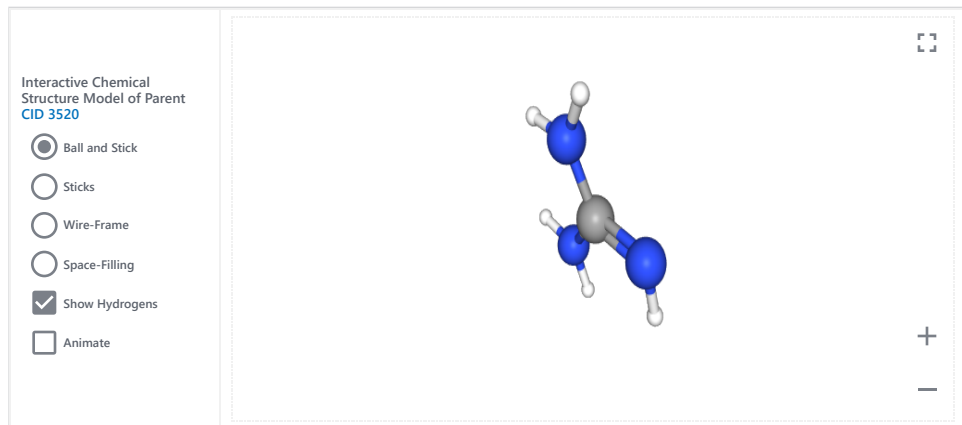
[from PubChem](#)

## 1.2 3D Conformer



### 3D Conformer of Parent

Get Image Download



## 2 Names and Identifiers



### 2.1 Computed Descriptors



#### 2.1.1 IUPAC Name



guanidine;hydrochloride

from PubChem

#### 2.1.2 InChI



InChI=1S/CH<sub>5</sub>N<sub>3</sub>.ClH/c2-1(3)4;/h(H5,2,3,4);1H

from PubChem

#### 2.1.3 InChI Key



PJJJBJSCAKJQF-UHFFFAOYSA-N

from PubChem

#### 2.1.4 Canonical SMILES



C(=N)(N)N.Cl

from PubChem

## 2.2 Molecular Formula



CH<sub>5</sub>ClN<sub>3</sub>

CH<sub>5</sub>N<sub>3</sub>.ClH

from ILO International Chemical Safety Cards (ICSC)

CH<sub>5</sub>ClN<sub>3</sub>

from PubChem

## 2.3 Other Identifiers



### 2.3.1 CAS



50-01-1

from ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); ILO International Chemical Safety Cards (ICSC); The National Institute for Occupational Safety and Health (NIOS)

#### Related CAS

113-00-8 (Parent)

from ChemIDplus

**Other CAS**

106946-18-3  
 139693-44-0  
 14317-32-9  
 143504-22-7  
 15827-40-4  
 420-13-3  
 87667-20-7  
 94369-44-5  
 915070-50-7  
 1340579-42-1

▶ from ChemDplus

**2.3.2 European Community (EC) Number**

200-002-3

▶ from European Chemicals Agency (ECHA)

**2.3.3 ICSC Number**

0894

▶ from ILO International Chemical Safety Cards (ICSC)

**2.3.4 NSC Number**

755884

▶ from DTP/NCI

**2.3.5 RTECS Number**

MF430000

▶ from The National Institute for Occupational Safety and Health (NIOSH)

**2.3.6 UNII**

3YQC9ZY4YB

▶ from FDA/SPL Indexing Data

**2.3.7 Wikipedia**

Guanidine hydrochloride

▶ from Wikipedia

**2.4 Synonyms****2.4.1 MeSH Entry Terms**

Chloride, Guanidinium	Guanidine Sulfite (1:1)
Chloride, Guanidium	Guanidinium
Guanidine	Guanidinium Chloride
Guanidine Hydrochloride	Guanidium Chloride
Guanidine Monohydrate	Hydrochloride, Guanidine
Guanidine Monohydrobromide	Monohydrate, Guanidine
Guanidine Monohydrochloride	Monohydrobromide, Guanidine
Guanidine Monohydroiodine	Monohydrochloride, Guanidine
Guanidine Nitrate	Monohydroiodine, Guanidine
Guanidine Phosphate	Nitrate, Guanidine
Guanidine Sulfate	Phosphate, Guanidine
Guanidine Sulfate (1:1)	Sulfate, Guanidine
Guanidine Sulfate (2:1)	

▶ from MeSH

**2.4.2 Depositor-Supplied Synonyms**

Guanidine hydrochloride 50-01-1	UNII-3YQC9ZY4YB Guanidium chloride	Guanidine hydrochloride, 99.5%, without anticaking agent guanidine-hcl
------------------------------------	---------------------------------------	---

Guanidinium chloride	USAF EK-749	CCRIS 8910
guanidine HCl	Guanidine, hydrochloride (1:1)	Guanidine hydrochloride, 98%, with <0.4% anticaking agent
Guanidine, monohydrochloride	EINECS 200-002-3	Guanidine.HCl
Aminoformamidine hydrochloride	MFC00013026	NIEaeO
Aminomethanamidine hydrochloride	3YQC9ZY4YB	eONIEaNI
GUANIDINE MONOHYDROCHLORIDE	AI3-19014	guanidine HCl salt
Guanidine chloride	Guanidine Hydrochloride, ULTROL&reg; Grade	Aminoformamidine HCl
Iminourea hydrochloride	Guanidinehydrochloride	qKxPSDQBBSP@
Carbamidine hydrochloride	Guanidine hydrochloride, >=98%	guanidine hydrochloride
Guanidinium hydrochloride	CHEBI:32735	Guanidine hydrochloride
Guanidine (hydrochloride)	GUANIDINE HYDROCHLORIDE, ULTRA PURE	Guanidine hydrochloride

▶ from PubChem

### 3 Chemical and Physical Properties



#### 3.1 Computed Properties



Property Name	Property Value
Molecular Weight	95.53 g/mol
Hydrogen Bond Donor Count	4
Hydrogen Bond Acceptor Count	1
Rotatable Bond Count	0
Exact Mass	95.025025 g/mol
Monoisotopic Mass	95.025025 g/mol
Topological Polar Surface Area	75.9 A^2
Heavy Atom Count	5
Formal Charge	0
Complexity	26.3
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

#### 3.2 Experimental Properties



##### 3.2.1 Physical Description



DryPowder; DryPowder, Liquid

▶ from EPA Chemicals under the TSCA

HYGROSCOPIC CRYSTALLINE POWDER.

▶ from ILO International Chemical Safety Cards (ICSC)

##### 3.2.2 Melting Point



182.3°C

▶ from EPA DSSTox

178-185 °C

▶ from ILO International Chemical Safety Cards (ICSC)

##### 3.2.3 Solubility



Solubility in water, g/100ml at 20 °C: 215

▶ from ILO International Chemical Safety Cards (ICSC)

##### 3.2.4 Density



1.3 g/cm<sup>3</sup>

▶ from ILO International Chemical Safety Cards (ICSC)

### 3.2.5 Octanol/Water Partition Coefficient



#### LogP

-1.7

▶ from ILO International Chemical Safety Cards (ICSC)

## 4 Spectral Information



### 4.1 1D NMR Spectra



#### 4.1.1 1H NMR Spectra



Instrument Name	Varian CFT-20
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

#### 4.1.2 13C NMR Spectra



Source of Sample	Fluka AG, Buchs, Switzerland
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	The Matheson Company, Inc.
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	



▶ from SpectraBase

Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Copyright	Copyright © 1980, 1981-2018 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



3520

▶ from PubChem

### 5.3 Related Compounds



Same Connectivity	5 Records
Same Parent, Connectivity	68 Records
Same Parent, Exact	52 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	21 Records

▶ from PubChem

### 5.4 Substances



### 5.4.1 Related Substances



Same	139 Records
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▶ from PubChem

### 5.4.2 Substances by Category



▶ from PubChem

## 6 Chemical Vendors



▶ from PubChem

## 7 Drug and Medication Information



### 7.1 FDA Orange Book



▶ from FDA Orange Book

### 7.2 Drug Labels for Ingredients



Label Title	GUANIDINE HYDROCHLORIDE- guanidine hydrochloride tablet
Drug Ingredient	GUANIDINE HYDROCHLORIDE
Label Image	

Label Download	<a href="#">PDF Label</a>
NDC Code(s)	0085-0492-01
Packager	Merck Sharp & Dohme Corp.

▶ from DailyMed

## 8 Pharmacology and Biochemistry ?

### 8.1 Pharmacology ?

Guanidine Hydrochloride is the hydrochloride salt form of [guanidine](#), a strong basic compound with parasymphomimetic activity. Guanidine hydrochloride enhances the release of [acetylcholine](#) following a nerve impulse and potentiates [acetylcholine](#) actions on muscarinic and nicotinic receptors. It also appears to slow the rates of depolarization and repolarization of muscle cell membranes. (NCI05)

▶ from NCI

## 9 Use and Manufacturing ?

### 9.1 Uses ?

EPA CPDat Chemical and Product Categories

▶ from EPA Chemical and Products Database (CPDat)

#### 9.1.1 Industry Uses ?

Flame retardants  
Laboratory chemicals  
Plating agents and surface treating agents  
Processing aids, not otherwise listed  
Protein Purification  
used as a purification reagent

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

▶ from EPA Chemicals under the TSCA

#### 9.1.2 Consumer Uses ?

Personal care products  
purification of protein

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

▶ from EPA Chemicals under the TSCA



## 9.2 U.S. Production ? ↗

### Aggregated Product Volume (EPA CDR 2016)

100,000 - 500,000 lb

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

▶ from EPA Chemicals under the TSCA

## 9.3 General Manufacturing Information ? ↗

### Industry Processing Sectors

Metal treatment  
Pharmaceutical and medicine manufacturing  
Textiles, apparel, and leather manufacturing  
Wholesale and retail trade  
biotechnology

▶ from EPA Chemicals under the TSCA

### EPA TSCA Commercial Activity Status

Guanidine, hydrochloride (1:1): ACTIVE

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


▶ from EPA Chemicals under the TSCA

## 10 Safety and Hazards ? ↗

### 10.1 Hazards Identification ? ↗

#### 10.1.1 GHS Classification ? ↗

Showing 1 of 4 [View More](#) ↗

Pictogram(s)	 Irritant
Signal	<b>Warning</b>
GHS Hazard Statements	H302: Harmful if swallowed [ <b>Warning</b> Acute toxicity, oral] H315: Causes skin irritation [ <b>Warning</b> Skin corrosion/irritation] H319: Causes serious eye irritation [ <b>Warning</b> Serious eye damage/eye irritation]
Precautionary Statement Codes	P264, P270, P280, P301+P312, P302+P352, P305+P351+P338, P321, P330, P332+P313, P337+P313, P362, and P501 (The corresponding statement to each P-code can be found at the <a href="#">GHS Classification</a> page.)

▶ from EU REGULATION (EC) No 1272/2008

#### 10.1.2 Fire Hazard ? ↗

Combustible.

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.2 First Aid Measures ? ↗

### 10.2.1 Inhalation First Aid ? ↗

Fresh air, rest.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.2.2 Skin First Aid ? ↗

Rinse skin with plenty of **water** or shower.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.2.3 Eye First Aid ? ↗

First rinse with plenty of **water** for several minutes (remove contact lenses if easily possible), then refer for medical attention.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.2.4 Ingestion First Aid



Rinse mouth. Give one or two glasses of [water](#) to drink. Induce vomiting (ONLY IN CONSCIOUS PERSONS!).

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.3 Fire Fighting



Use foam, powder.

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.4 Accidental Release Measures



### 10.4.1 Spillage Disposal



Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of [water](#). Personal protection: P2 filter respirator for harmful particles.

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.5 Handling and Storage



### 10.5.1 Safe Storage



Well closed. Dry.

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.6 Exposure Control and Personal Protection



### 10.6.1 Inhalation Risk



Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.2 Effects of Short Term Exposure



The substance is irritating to the eyes and skin.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.3 Fire Prevention



NO open flames.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.4 Exposure Prevention



PREVENT DISPERSION OF DUST!

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.5 Inhalation Prevention



Use local exhaust or breathing protection.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.6 Skin Prevention



Protective gloves. Protective clothing.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.7 Eye Prevention



Wear safety goggles or eye protection in combination with breathing protection.

▶ from ILO International Chemical Safety Cards (ICSC)

### 10.6.8 Ingestion Prevention



Do not eat, drink, or smoke during work.

▶ from ILO International Chemical Safety Cards (ICSC)

## 10.7 Transport Information



### 10.7.1 EC Classification



Symbol: Xn; R: 22-36/38; S: (2)-22

▶ from ILO International Chemical Safety Cards (ICSC)

## 11 Toxicity



### 11.1 Toxicological Information



#### 11.1.1 NIOSH Toxicity Data



▶ from The National Institute for Occupational Safety and Health (NIOSH)

#### 11.1.2 Exposure Routes



The substance can be absorbed into the body by ingestion.

▶ from ILO International Chemical Safety Cards (ICSC)

#### 11.1.3 Inhalation Symptoms



Cough.

▶ from ILO International Chemical Safety Cards (ICSC)

#### 11.1.4 Skin Symptoms



Redness.

▶ from ILO International Chemical Safety Cards (ICSC)

#### 11.1.5 Eye Symptoms



Redness. Pain.

▶ from ILO International Chemical Safety Cards (ICSC)

#### 11.1.6 Ingestion Symptoms



Diarrhoea.

▶ from ILO International Chemical Safety Cards (ICSC)

#### 11.1.7 Acute Effects



▶ from ChemIDplus

### 11.1.8 US EPA Regional Screening Levels for Chemical Contaminants



Resident Soil (mg/kg)	1.3E+02
Industrial Soil (mg/kg)	1.6E+03
Tapwater (ug/L)	4.0E+01

▶ from US EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

## 12 Literature



### 12.1 NLM Curated PubMed Citations



▶ from PubChem

### 12.2 Springer Nature References



▶ from Springer Nature

### 12.3 Thieme References



▶ from Thieme Chemistry

## 12.4 Chemical Co-Occurrences in Literature

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▶ from PubChem

## 12.5 Chemical-Disease Co-Occurrences in Literature

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▶ from PubChem

## 12.6 Chemical-Gene Co-Occurrences in Literature

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▶ from PubChem

## 13 Patents

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### 13.1 Depositor-Supplied Patent Identifiers

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▶ from PubChem

## 14 Biological Test Results



### 14.1 BioAssay Results



▶ from PubChem

## 15 Classification



### 15.1 Ontologies



#### 15.1.1 MeSH Tree



▶ from MeSH

#### 15.1.2 WIPO IPC



▶ from WIPO

### 15.1.3 ChemIDplus



▶ from ChemIDplus

### 15.1.4 UN GHS Classification



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

### 15.1.5 EPA CPDat Classification



▶ from EPA Chemical and Products Database (CPDat)

## 16 Information Sources



FILTER BY SOURCE

#### 1. ChemIDplus

Guanidine hydrochloride

<https://chem.nlm.nih.gov/chemidplus/sid/0000050011>

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

## 2. DTP/NCI

Guanidine hydrochloride  
<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=755884>

## 3. EPA Chemicals under the TSCA

Guanidine, hydrochloride (1:1)  
<https://www.epa.gov/chemicals-under-tsca>

## 4. EPA DSSTox

Guanidine monohydrochloride  
<https://comptox.epa.gov/dashboard/DTXSID7058757>

## 5. European Chemicals Agency (ECHA)

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

Guanidinium chloride  
<https://echa.europa.eu/substance-information/-/substanceinfo/100.000.003>

Guanidinium chloride  
<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/52449>

## 6. ILO International Chemical Safety Cards (ICSC)

GUANIDINE HYDROCHLORIDE  
[http://www.ilo.org/dyn/cscs/showcard.display?p\\_version=2&p\\_card\\_id=0894](http://www.ilo.org/dyn/cscs/showcard.display?p_version=2&p_card_id=0894)

## 7. The National Institute for Occupational Safety and Health (NIOSH)

Guanidine, monohydrochloride  
<https://www.cdc.gov/niosh-rtecs/MF419CE0.html>

## 8. DailyMed

GUANIDINE HYDROCHLORIDE  
<https://dailymed.nlm.nih.gov/dailymed/search.cfm?labeltype=all&query=GUANIDINE+HYDROCHLORIDE>

## 9. EPA Chemical and Products Database (CPDat)

guanidine hydrochloride  
<https://comptox.epa.gov/dashboard/DTXSID7058757#exposure>  
EPA CPDat Classification  
<https://www.epa.gov/chemical-research/chemical-and-products-database-cpd>

## 10. EU REGULATION (EC) No 1272/2008

guanidinium chloride;guanadine hydrochloride  
[https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv%3AAOJ.L\\_2018.115.01.0001.01.ENG](https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv%3AAOJ.L_2018.115.01.0001.01.ENG)

## 11. Hazardous Chemical Information System (HCIS), Safe Work Australia

guanidinium chloride  
<http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=2341>

## 12. NITE-CMC

guanidinium chloride; guanadine hydrochloride  
<http://www.safe.nite.go.jp/english/ghs/08-mhlw-0067e.html>

## 13. FDA Orange Book

<https://www.fda.gov/Drugs/InformationOnDrugs/ucm129662.htm>

## 14. FDA/SPL Indexing Data

3YQC9ZY4YB  
<https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/>

## 15. NCI

Guanidine Hydrochloride  
[https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI\\_Thesaurus&ns=NCI\\_Thesaurus&code=C47551](https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C47551)

## 16. SpectraBase

<https://spectrabase.com/spectrum/HcDV9G9hI48>  
<https://spectrabase.com/spectrum/32vV48LDjvw>  
<https://spectrabase.com/spectrum/57zW6saWBEK>  
<https://spectrabase.com/spectrum/FLualZ6py0i>

## 17. Springer Nature

## 18. Thieme Chemistry

## 19. US EPA Regional Screening Levels for Chemical Contaminants at Superfund Sites

Guanidine Chloride  
[https://epa-prgs.oml.gov/cgi-bin/chemicals/csl\\_search](https://epa-prgs.oml.gov/cgi-bin/chemicals/csl_search)

## 20. Wikipedia

guanidine hydrochloride  
[https://en.wikipedia.org/wiki/Guanidinium\\_chloride](https://en.wikipedia.org/wiki/Guanidinium_chloride)

## 21. MeSH

Guanidine  
<https://www.ncbi.nlm.nih.gov/mesh/68019791>  
MeSH Tree  
<http://www.nlm.nih.gov/mesh/meshhome.html>

## 22. PubChem

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



23. **WIPO**

*International Patent Classification*

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

24. **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)