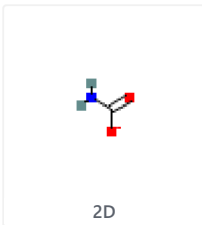
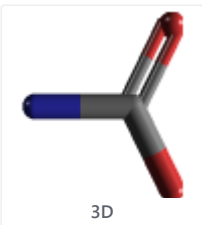
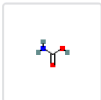


## COMPOUND SUMMARY

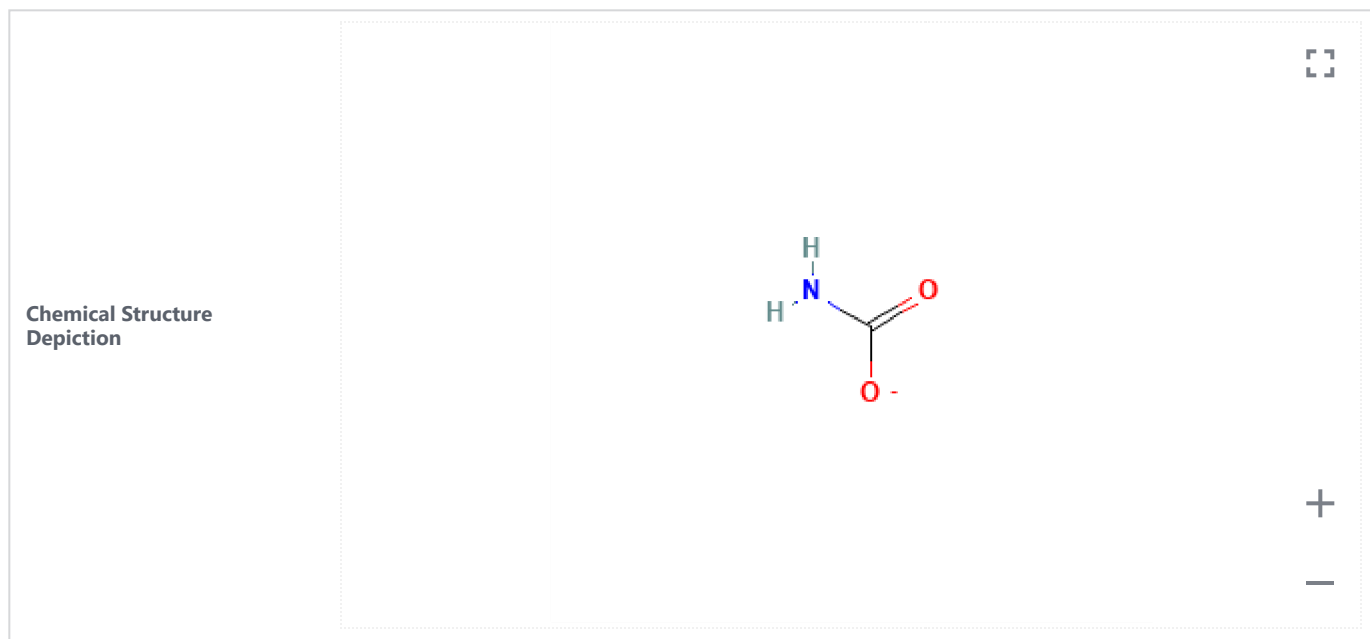
# Carbamate

<b>PubChem CID</b>	276				
<b>Structure</b>	<div style="display: flex; justify-content: space-around; align-items: center;"> <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>	CH <sub>2</sub> NO <sub>2</sub> <sup>-</sup>				
<b>Synonyms</b>	carbamate Carbamate ion Carbamic acid, ion(1-) 302-11-4 Carbamates <input type="button" value="More..."/>				
<b>Molecular Weight</b>	60.032				
<b>Parent Compound</b>	 <a href="#">CID 277 (Carbamic acid)</a>				
<b>Dates</b>	<table style="width: 100%; border: none;"> <tr> <td style="width: 50%;">Modify</td> <td style="width: 50%;">Create</td> </tr> <tr> <td>2022-08-27</td> <td>2005-06-23</td> </tr> </table>	Modify	Create	2022-08-27	2005-06-23
Modify	Create				
2022-08-27	2005-06-23				
<p>Carbamate is an amino-acid anion. It is a conjugate base of a <a href="#">carbamic acid</a>.</p> <p><a href="#">▶ ChEBI</a></p> <p>Derivatives of carbamic acid, H<sub>2</sub>NC(=O)OH. Included under this heading are N-substituted and O-substituted carbamic acids. In general carbamate esters are referred to as urethanes, and polymers that include repeating units of carbamate are referred to as POLYURETHANES. Note however that polyurethanes are derived from the polymerization of ISOCYANATES and the singular term URETHANE refers to the ethyl ester of carbamic acid.</p> <p><a href="#">▶ Medical Subject Headings (MeSH)</a></p>					

# 1 Structures



## 1.1 2D Structure



▶ [PubChem](#)

## 1.2 3D Conformer



▶ [PubChem](#)

## 2 Names and Identifiers

### 2.1 Computed Descriptors

#### 2.1.1 IUPAC Name

carbamate

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

[▶ PubChem](#)

#### 2.1.2 InChI

InChI=1S/CH<sub>3</sub>NO<sub>2</sub>/c2-1(3)4/h2H<sub>2</sub>, (H,3,4)/p-1

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

[▶ PubChem](#)

#### 2.1.3 InChIKey

KXDHJXZQYSOELW-UHFFFAOYSA-M

*Computed by InChI 1.0.6 (PubChem release 2021.05.07)*

[▶ PubChem](#)

#### 2.1.4 Canonical SMILES

C(=O)(N)[O-]

*Computed by OEChem 2.3.0 (PubChem release 2021.05.07)*

[▶ PubChem](#)

## 2.2 Molecular Formula

CH<sub>2</sub>NO<sub>2</sub>-

*Computed by PubChem 2.1 (PubChem release 2021.05.07)*

[▶ PubChem](#)

## 2.3 Other Identifiers

### 2.3.1 CAS

302-11-4

[▶ CAS Common Chemistry; ChemIDplus; EPA DSSTox](#)

### 2.3.2 DSSTox Substance ID

DTXSID80184291

[▶ EPA DSSTox](#)

### 2.3.3 Wikidata



Q27108972

[▶ Wikidata](#)

## 2.4 Synonyms



### 2.4.1 MeSH Entry Terms



Acids, Aminoformic  
 Acids, Carbamic  
 Aminoformic Acids  
 Carbamate  
 Carbamates  
 Carbamic Acids

[▶ Medical Subject Headings \(MeSH\)](#)

### 2.4.2 Depositor-Supplied Synonyms



carbamate	7224-09-1
Carbamate ion	Q27108972
Carbamic acid, ion(1-)	
302-11-4	
Carbamates	
carboxamide	
Carbamat	
Karbamat	
carboxy-amide	
racemic carbamate	
Carbamic acid anion	
CHEBI:13941	
DTXSID80184291	

[▶ PubChem](#)

## 3 Chemical and Physical Properties



### 3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	60.032	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	-0.1	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	0	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	60.008553307	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	60.008553307	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	66.2 Å <sup>2</sup>	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	4	Computed by PubChem
Formal Charge	-1	Computed by PubChem
Complexity	27.5	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	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

► [PubChem](#)

## 4 Related Records

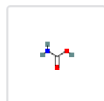


### 4.1 Related Compounds with Annotation



▶ PubChem

### 4.2 Parent Compound



CID 277 (Carbamic acid)

▶ PubChem

### 4.3 Related Compounds



Same Connectivity	2 Records
Same Parent, Connectivity	198 Records
Same Parent, Exact	191 Records
Mixtures, Components, and Neutralized Forms	1 Record
Similar Compounds	26 Records
Similar Conformers	111 Records

▶ PubChem

### 4.4 Substances



#### 4.4.1 Related Substances



Same	28 Records
------	------------

[▶ PubChem](#)

## 4.4.2 Substances by Category

[▶ PubChem](#)

## 4.5 Entrez Crosslinks



<b>PubMed</b>	<a href="#">21 Records</a>
<b>Taxonomy</b>	<a href="#">3 Records</a>
<b>OMIM</b>	<a href="#">3 Records</a>
<b>Gene</b>	<a href="#">23 Records</a>

[▶ PubChem](#)

## 5 Pharmacology and Biochemistry

---



### 5.1 Biochemical Reactions

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▶ [Rhea - Annotated Reactions Database](#)

▶ [PubChem](#)



## 6 Associated Disorders and Diseases

---



▶ [Comparative Toxicogenomics Database \(CTD\)](#)

## 7 Literature

---



### 7.1 NLM Curated PubMed Citations

---



▶ PubChem

### 7.2 Thieme References

---



▶ Thieme Chemistry

### 7.3 Depositor Provided PubMed Citations

---



▶ PubChem

## 7.4 Chemical Co-Occurrences in Literature

---



▶ PubChem

## 7.5 Chemical-Gene Co-Occurrences in Literature

---



▶ PubChem

## 7.6 Chemical-Disease Co-Occurrences in Literature

---



▶ PubChem

## 8 Patents



### 8.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

### 8.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

▶ PATENTSCOPE (WIPO)

## 9 Biomolecular Interactions and Pathways



### 9.1 Chemical-Gene Interactions



#### 9.1.1 CTD Chemical-Gene Interactions



▶ [Comparative Toxicogenomics Database \(CTD\)](#)

## 9.2 Pathways



▶ [PubChem](#)

## 10 Classification



### 10.1 MeSH Tree



► Medical Subject Headings (MeSH)

### 10.2 ChEBI Ontology



► ChEBI

### 10.3 ChemIDplus



► ChemIDplus

## 10.4 NORMAN Suspect List Exchange Classification

---



► NORMAN Suspect List Exchange

## 10.5 EPA DSSTox Classification

---





▶ EPA DSSTox

# 11 Information Sources



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## 1. CAS Common Chemistry

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*Carbamic acid, ion(1-)*

[https://commonchemistry.cas.org/detail?cas\\_rn=302-11-4](https://commonchemistry.cas.org/detail?cas_rn=302-11-4)

## 2. ChemIDplus

### LICENSE

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

*Carbamic acid, ion(1-)*

<https://chem.nlm.nih.gov/chemidplus/sid/0000302114>

ChemIDplus Chemical Information Classification

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

## 3. EPA DSSTox

### LICENSE

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

*Carbamic acid, ion(1-)*

<https://comptox.epa.gov/dashboard/DTXSID80184291>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

## 4. ChEBI

Carbamate

<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:13941>

ChEBI Ontology

<http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology>

## 5. Comparative Toxicogenomics Database (CTD)

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<http://ctdbase.org/about/legal.jsp>

<https://ctdbase.org/detail.go?type=chem&acc=D002219>

## 6. Rhea - Annotated Reactions Database

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<https://www.rhea-db.org/rhea?query=CHEBI:13941>

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## 8. Wikidata

## LICENSE

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