

 Compound Summary for CID 10130287

PUBCHEM &gt; COMPOUND &gt; CALCIUM GLYCINATE

# Calcium Glycinate

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Vendors



Patents

**PubChem CID:** 10130287

Calcium glycinate; 35947-07-0; UNII-567R60Z85R; Calcium glycine;

**Chemical Names:**

567R60Z85R; 56-40-6 (Parent);

[More...](#)**Molecular Formula:**  $C_4H_8CaN_2O_4$ **Molecular Weight:** 188.19532 g/mol**InChI Key:** OFNJDDJDXNMTHZ-UHFFFAOYSA-L**Modify Date:** 2016-06-11**Create Date:** 2006-10-25

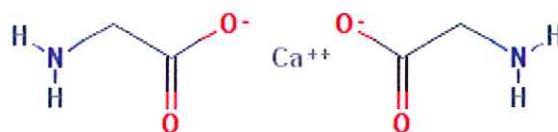
## 1 2D Structure



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### 3 Names and Identifiers



#### 3.1 Computed Descriptors



##### 3.1.1 IUPAC Name



calcium;2-aminoacetate

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##### 3.1.2 InChI



InChI=1S/2C2H5NO2.Ca/c2\*3-1-2(4)5;/h2\*1,3H2,(H,4,5);/q;+2/p-2

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##### 3.1.3 InChI Key



OFNJDDJDXNMTHZ-UHFFFAOYSA-L

▶ from PubChem

##### 3.1.4 Canonical SMILES



C(C(=O)[O-])N.C(C(=O)[O-])N.[Ca+2]

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#### 3.2 Molecular Formula



C4H8CaN2O4

▶ from PubChem

#### 3.3 Other Identifiers



##### 3.3.1 EC Number



252-809-5

▶ from ECHA

251-422-9

▶ from ECHA

#### 3.4 Synonyms



##### 3.4.1 Depositor-Supplied Synonyms



- |                            |                                  |                |
|----------------------------|----------------------------------|----------------|
| 1. Calcium glycinate       | 11. calcium 2-azanylethanoate    | 21. P522       |
| 2. 35947-07-0              | 12. C4H8CaN2O4                   | 22. A823056    |
| 3. UNII-567R60Z85R         | 13. Calcium glycinate (1:2)      | 23. I14-8085   |
| 4. calcium glycine         | 14. SCHEMBL344659                | 24. 33242-26-1 |
| 5. 567R60Z85R              | 15. Jsp006436                    |                |
| 6. 56-40-6 (Parent)        | 16. CTK1C2294                    |                |
| 7. Calcium 2-aminoacetate  | 17. OFNJDDJDIXNMTHZ-UHFFFAOYSA-L |                |
| 8. Calciumglycinate        | 18. EINECS 251-422-9             |                |
| 9. calcium bisglycinate    | 19. EINECS 252-809-5             |                |
| 10. Diglycine calcium salt | 20. AKOS015918298                |                |

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## 4 Chemical and Physical Properties



### 4.1 Computed Properties



Molecular Weight	188.19532 g/mol
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	6
Rotatable Bond Count	0
Exact Mass	188.010998 g/mol
Monoisotopic Mass	188.010998 g/mol
Topological Polar Surface Area	132 A <sup>2</sup>
Heavy Atom Count	11
Formal Charge	0
Complexity	37.4
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	3

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