## **Phenylacetic acid**

| Phenylacetic acid   |  |                        |
|---|--|------------------------|
| [[Image:Kwas fenylooctowy.svg   |  | Phenylacetic acid]]    |
| [[Image:Phenylacetic-acid-3D-balls-B.png  |  | Ball-and-stick model]] |
| Identifiers   |  |                        |
| CAS number  | 103-82-2 [1] 🗸                               |                        |
| ChemSpider  | 10181341 [2] 🗸                               |                        |
| UNII  | ER5I1W795A <sup>[3]</sup> 🗸                  |                        |
| ChEMBL  | CHEMBL1044 <sup>[4]</sup> 🗸                  |                        |
| Jmol-3D images  | Image 1 <sup>[5]</sup>                       |                        |
| Properties  |  |                        |
| Molecular formula   | C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> |                        |
| Molar mass  | 136.15 g/mol                                 |                        |
| Density   | 1.0809 g/cm <sup>3</sup>                     |                        |
| Melting point   | 76-77 °C                                     |                        |
| Boiling point   | 265.5 °C                                     |                        |
| Acidity (pK <sub>a</sub> )  | 4.31 <sup>[6]</sup>                          |                        |
| Hazards   |  |                        |
| MSDS  | External MSDS <sup>[7]</sup>                 |                        |
| (what is this?) (verify) <sup>[8]</sup><br>Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa) |  |                        |
| Infobox references  |  |                        |

**Phenylacetic acid** (abr. **PAA** and synonyms are:  $\alpha$ -toluic acid, benzeneacetic acid, alpha tolylic acid, **2-phenylacetic acid**) is an organic compound containing a phenyl functional group and a carboxylic acid functional group. It is a white solid with a disagreeable odor. Because it is used in the illicit production of phenylacetone (used in the manufacture of meth/amphetamines), it is subject to controls in the United States.

#### Occurrence

Phenylacetic acid has been found to be an active auxin (a type of plant hormone),<sup>[9]</sup> predominantly found in fruits. However its effect is much weaker than the effect of the basic auxin molecule indole-3-acetic acid. It is also the oxidation product of phenethylamine when acted on by the enzyme monoamine oxidase found in humans and many other organisms.

### Preparation

This compound may be prepared by the hydrolysis of benzyl cyanide:<sup>[10] [11]</sup>



### Applications

References

Phenylacetic acid is used in some perfumes, possessing a honey-like odour in low concentrations, and is also used in penicillin G production. It is also employed to treat type II hyperammonemia to help reduce the amounts of ammonia in a patient's bloodstream by forming phenylacetyl-CoA which then reacts with nitrogen-rich glutamine to form phenylacetylglutamine. This compound is then secreted by the patient's body.

-NH₄CI



### [1] http://www.commonchemistry.org/ChemicalDetail.aspx?ref=103-82-2

- [2] http://www.chemspider.com/10181341
- [3] http://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=ER5I1W795A
- [4] https://www.ebi.ac.uk/chembldb/index.php/compound/inspect/CHEMBL1044
- [5] http://chemapps.stolaf.edu/jmol/jmol.php?model=O%3DC%28O%29Cc1ccccc1
- [6] Dippy, J.F.J., Hughes, S.R.C., Rozanski, A., J. Chem Soc., 1959, 2492.
- [7] http://ptcl.chem.ox.ac.uk/MSDS/PH/phenylacetic\_acid.html
- [8] http://en.wikipedia.org/wiki/%3Aphenylacetic\_acid?diff=cur&oldid=417793686
- [9] Wightman, Frank; Lighty, Douglas L. (1982). "Identification of phenylacetic acid as a natural auxin in the shoots of higher plants". *Physiologia Plantarum* 55 (1): 17. doi:10.1111/j.1399-3054.1982.tb00278.x.
- [10] Roger Adams; A. F. Thal (1941), "Phenylacetic acid" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv1p0436), Org. Synth., ; Coll. Vol. 1: 436
- [11] Wilhelm Wenner (1963), "Phenylacetamide" (http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv4p0760), Org. Synth., ; Coll. Vol. 4: 760

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