

PRODUCT CODE- PMPYAA487



Taj Pharmaceuticals Ltd.

Para Methoxy Phenyl Acetic Acid

**CAS No. 104-01-8**



48705152689765500106

## Para Methoxy Phenyl Acetic Acid

### IUPAC Name:

2-(4-methoxyphenyl)acetic acid

### Synonyms:

Homoanisic acid, Benzeneacetic acid, 4-methoxy-, p-Methoxyphenylacetic acid, 2-(p-Anisyl)acetic acid, MOPA, 4-Methoxyphenylacetic acid, 4-Methoxybenzeneacetic acid, (4-Methoxyphenyl)acetic acid, Acetic acid, (p-methoxyphenyl)-, Acetic acid, p-methoxyphenyl-, WLN: QV1R DO1, NCIOpen2\_000187, (p-Methoxyphenyl)acetic acid, M19201\_ALDRICH, EINECS 203-166-4, NSC 27799, AIDS017837, P-METHOXYPHENYLACETIC ACID, AIDS-017837, NSC27799

CAS Registry Number: 104-01-8

Molecular Formula: C<sub>9</sub>H<sub>10</sub>O<sub>3</sub>

Molecular Weight: 166.173900 [g/mol]

H-Bond Donor: 1 H-Bond Acceptor: 3

Melting Point : 84-86 °C(lit.)

Boiling Point : 140 °C3 mm Hg(lit.)

Fp : 193°C

Water Solubility : 6 g/L (20 °C)

TOXICITY

Oral rat LD50: 1550 mg/Kg

STABILITY : Stable under ordinary conditions

### DESCRIPTION & APPLICATIONS

Phenylacetic acid is a white crystals with a disagreeable odor; boiling point 262 C; soluble in alcohol and ether. It serves as an ingredient in perfume to provide honey-like odor. It is found as a moiety in some alkaloids and plant hormones. It is formed as catabolite of phenylalanine. Substituted phenylacetic acid molecule at alpha position and phenylacetate esters can serve as a drug with a wide variety of effects including anticholinergic, muscarinic antagonist, antidote to cholinesterase inhibitors or toxins, cycloplegic and mydriatic. Phenylacetic acid is used to prepare a nonsteroidal antiinflammatory drug like diclofenac. It is used the manufacture of penicillin. Mandelic Acid, phenylglycollic acid, can be produced from phenylchloroacetic acid.

4-Methoxyphenylacetic Acid is used as an intermediate for pharmaceuticals (especially for dextromethorphan) and other organic synthesis. It is used as a plant growth regulator and herbicide.

### SPECIFICATION

APPEARANCE white to off-white powder

ASSAY 99.0% min

CLARITY IN ETHANOL clear



Taj Group of Companies

**TAJ PHARMACEUTICALS LIMITED**<sup>INDIA</sup>

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### Phenylacetic acid definition - medical

An abnormal product of phenylalanine catabolism that appears in the urine in phenylketonuria.

### Synthesis of Phenylacetic Acid

#### Phenylacetic Acid from Benzyl Chloride

10% of a solution of 125 g benzyl chloride [1] in 250 ml of sodium-distilled diethyl ether is added to 24 g magnesium turnings under 100 ml ether, and a small iodine crystal is added. After start of the Grignard reaction the rest of the benzyl chloride is added with stirring to maintain gentle boiling (if the reaction becomes too vigorous, useless 1,2-diphenylethane is formed) and the mixture is heated and stirred until most magnesium is dissolved. The Grignard reagent solution is poured on 1 kg water-free, crushed dry ice (solid CO<sub>2</sub>) and stirred for 2 hrs. 200 ml warm ether is added and the mixture is heated in a water-bath until the internal temperature reaches 25°C. 200 ml 32% hydrochloric acid is added, and the heterogeneous mixture stirred until any inorganic precipitate is dissolved. After filtering, the organic layer is separated, washed with cold water, and dried over 20 g anhydrous sodium sulfate. The ether is distilled off, and the rest is recrystallized from water, to yield 75% - about 100g - phenylacetic acid, mp 76-77°C.

#### Phenylacetic acid from Benzyl Cyanide

In a silica basin of about 35 cm. diameter, a mixture of 2.5 kilos of benzyl cyanide [3] and 7.5 kilos of 70% sulfuric acid is warmed until a few bubbles of gas appear. The heating is at once stopped, since a very vigorous action now ensues. As the vapors evolved are injurious to health, the basin is covered when the reaction begins with a sliding cover from which the vapors can be led into water. As soon as the reaction ceases, the product is poured upon crushed ice in a large, earthenware vessel. Crude phenyl acetic acid, contaminated on the surface with phenyl acetamide, is precipitated on cooling. In order to remove the amide, the acid is dissolved in lukewarm dilute soda solution. The amide remains undissolved and can be filtered off, while the phenyl acetic acid goes into solution as sodium salt and is reprecipitated in a sufficiently pure state by the addition of dilute mineral acid. After drying it is acceptably pure.

This document plus the full buyer / prescribing information, prepared for health professionals can be found at:

<http://www.tajapi.com>

or by contacting the sponsor, Taj Pharmaceuticals Limited., at:

91 022 30601000.

This leaflet was prepared by  
Taj Pharmaceuticals Limited,  
Mumbai (India).

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