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Compound Summary for CID 999

Phenylacetic Acid

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999

PHENYLACETIC ACID; 2-Phenylacetic acid; Benzeneacetic acid; 103-82-2; Phenylethanoic acid;

Chemical Names:

PubChem CID:

Alpha-Toluic acid More...

Molecular Formula:

C8H8O2; C6H5CH2CO2H

Molecular Weight:

136.15 g/mol

InChl Key:

WLJVXDMOQOGPHL-UHFFFAOYSA-N

Drug Information:

Drug Indication

Clinical Trials FDA UNII

Safety Summary:

Laboratory Chemical Safety Summary (LCSS)

Phenylacetic acid is a Nitrogen Binding Agent. The mechanism of action of phenylacetic acid is as an Ammonium Ion Binding Activity.

▶ FDA Pharmacology Summary from FDA Pharm Classes

Phenyl acetate (or phenylacetate) is a carboxylic acid ester that has been found in the biofluids of patients with nephritis and/or hepatitis as well as patients with phenylketonuria (PKU), an inborn error of metabolism. Excess phenylalanine in the body can be disposed of through a transamination process leading to the production of phenylpyruvate. The phenylpyruvate can be further metabolized into a number of products. Decarboxylation of phenylpyruvate gives phenylacetate, while a reduction reaction gives phenyllactate. The phenylacetate can be further conjugated with glutamine to give phenylacetyl glutamine. All of these metabolites can be detected in serum and urine of PKU patients. Phenyl acetate is also produced endogenously as the metabolite of 2-Phenylethylamine, which is mainly metabolized by monoamine oxidase to form phenyl acetate. 2-phenylethylamine is an "endogenous amphetamine" which may modulate central adrenergic functions, and the urinary phenyl acetate levels have been postulated as a marker for depression. (PMID: 17978765, 476920, 6857245). Phenylacetate is also found in essential oils, e. g. neroli, rose oil, free and as esters' and in many fruits. As a result it is used as a perfumery and flavoring ingredient.

▶ Metabolite Description from Human Metabolome Database (HMDB)



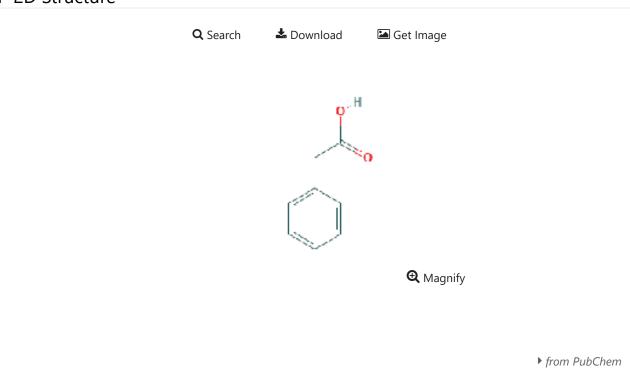


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1 2D Structure



2 3D Conformer

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