Compound Summary for CID 66827

Phenylboronic Acid

Cite this Record

STRUCTURE VENDORS PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	66827
Chemical Names:	Phenylboronic acid; 98-80-6; Benzeneboronic acid; Boronic acid, phenyl-; Phenylboric acid; Dihydroxyphenylborane More...
Molecular Formula:	$C_6H_7BO_2$
Molecular Weight:	121.93 g/mol
InChI Key:	HXITXNWTGFUOAU-UHFFFAOYSA-N
Substance Registry:	FDA UNII
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)

14-hydroperoxy-H4-neuroprostane, also known as Benzeneboronic acid or PHENYL boronate, is classified as a benzene or a Benzene derivative. Benzenes are aromatic compounds containing one monocyclic ring system consisting of benzene. 14-hydroperoxy-H4-neuroprostane is considered to be soluble (in water) and acidic. 14-hydroperoxy-H4-neuroprostane can be synthesized from boronic acid. 14-hydroperoxy-H4-neuroprostane can be synthesized into 4-fluorophenylboronic acid and 3-acetylphenylboronic acid.

Metabolite Description from Human Metabolome Database

PUBCHEM > COMPOUND > PHENYLBORONIC ACID *Create Date: 2005-03-26*

Contents

1 2D Structure
2 3D Status
3 Names and Identifiers
4 Chemical and Physical Properties
5 Related Records
6 Chemical Vendors
7 Pharmacology and Biochemistry
8 Safety and Hazards
9 Literature
10 Patents
11 Biomolecular Interactions and Pathways
12 Biological Test Results
13 Classification
14 Information Sources

1 2D Structure

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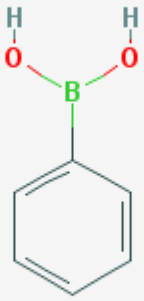

Magnify

from PubChem

2 3D Status

Conformer generation is disallowed since MMFF94s unsupported element

from PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

phenylboronic acid

from PubChem

3.1.2 InChI

InChI=1S/C6H7BO2/c8-7(9)6-4-2-1-3-5-6/h1-5,8-9H

from PubChem

3.1.3 InChI Key

HXITXNWTGFUOAU-UHFFFAOYSA-N

from PubChem

3.1.4 Canonical SMILES

B(C1=CC=CC=C1)(O)O

from PubChem

3.2 Molecular Formula

$C_6H_7BO_2$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

98-80-6

from ChemIDplus, European Chemicals Agency - ECHA, Human Metabolome Database

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