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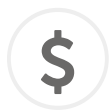
Search Compounds

 Compound Summary for CID 66827

Phenylboronic Acid

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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

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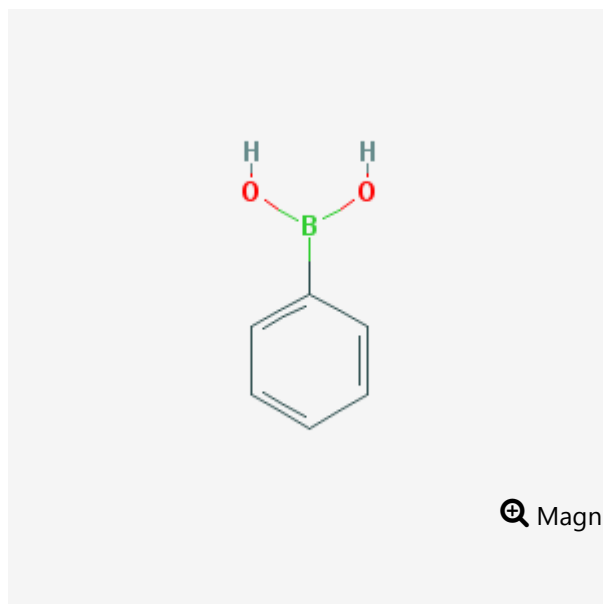
14 Information Sources

1 2D Structure

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▶ 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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