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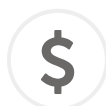


Compound Summary for CID 2775922

# 1582-24-7

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STRUCTURE



VENDORS



LITERATURE



PATENTS

**PubChem CID:**

2775922

**Chemical Names:**1582-24-7; 2,3,4,5,6-PENTAFLUOROBENZENE BORONIC ACID;  
Pentafluorophenylboronic acid; 2,3,4,5,6-PENTAFLUOROPHENYLBORONIC ACID;  
Pentafluorobenzeneboronic acid; Perfluorophenylboronic acid [More...](#)**Molecular Formula:** $C_6H_2BF_5O_2$ **Molecular Weight:**

211.882 g/mol

**InChI Key:**

VASOMTXTRMYSKD-UHFFFAOYSA-N

**Safety Summary:**[Laboratory Chemical Safety Summary \(LCSS\)](#)[PUBCHEM](#) > [COMPOUND](#) > 1582-24-7

Create Date: 2005-07-19

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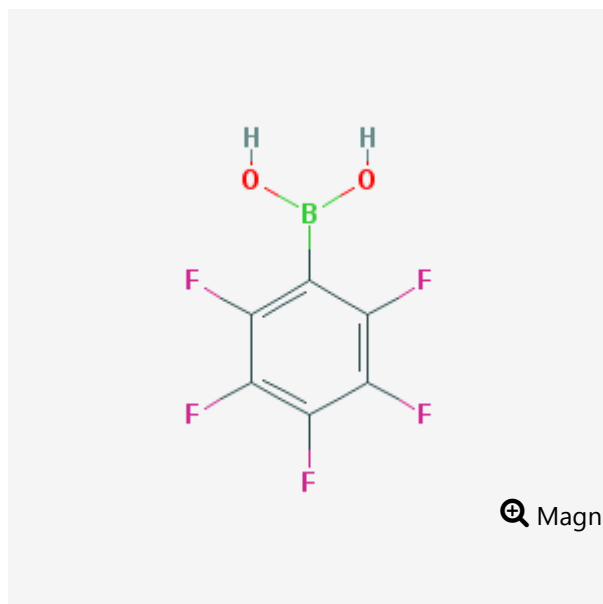
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## 1 2D Structure

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▶ *from PubChem*

## 2 3D Status

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Conformer generation is disallowed since MMFF94s unsupported element

▶ *from PubChem*

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## 3 Names and Identifiers

### 3.1 Computed Descriptors

#### 3.1.1 IUPAC Name

(2,3,4,5,6-pentafluorophenyl)boronic acid

▶ from PubChem

#### 3.1.2 InChI

InChI=1S/C6H2BF5O2/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h13-14H

▶ from PubChem

#### 3.1.3 InChI Key

VASOMTXTRMYSKD-UHFFFAOYSA-N

▶ from PubChem

#### 3.1.4 Canonical SMILES

B(C1=C(C(=C(C(=C1F)F)F)F)F)(O)O

▶ from PubChem

### 3.2 Molecular Formula

C<sub>6</sub>H<sub>2</sub>BF<sub>5</sub>O<sub>2</sub>

▶ from PubChem

### 3.3 Synonyms

#### 3.3.1 Depositor-Supplied Synonyms

- |                                             |                                               |
|---------------------------------------------|-----------------------------------------------|
| 1. 1582-24-7                                | 11. AK-44491                                  |
| 2. 2,3,4,5,6-PENTAFLUOROBENZENEBORONIC ACID | 12. BORONIC ACID, B-(2,3,4,5,6-PENTAFLUOROPHE |
| 3. Pentafluorophenylboronic acid            | 13. AC1MCQKY                                  |
| 4. 2,3,4,5,6-PENTAFLUOROPHENYL BORONIC ACID | 14. PubChem22760                              |

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