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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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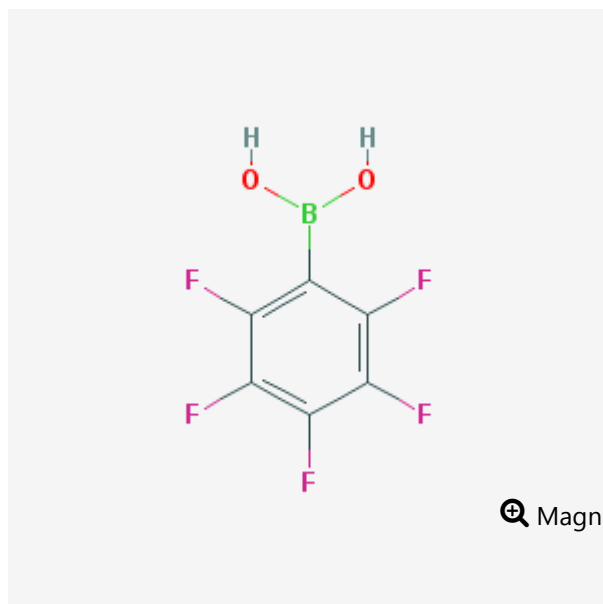
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1 2D Structure

[Search](#)[Download](#)[Get Image](#)[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

(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

$C_6H_2BF_5O_2$

▶ 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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