

HOW TO

Explore by Chemical Structure



With SciFinder[®], you can draw a chemical structure and then find a particular substance or group of substances that match the structure.

Exact search results may include:

- The structure exactly as you have drawn it
- Stereoisomers
- Tautomers (including keto-enol)
- Coordination compounds
- Charged compounds
- Radicals or radical ions
- Isotopes
- Polymers, mixtures, and salts

1. Click the structure drawing thumbnail to open the editor. You can toggle between the Structure and Reaction Drawing Editor.

Use the tools down the left side and across the bottom to draw your structure. Keyboard shortcut keys are also available.

Select **Exact search**, and click **OK**.

Tips:

- It may be helpful to set your browser to full screen when using the Structure Editor. You can also resize the window by dragging its lower-right corner.
- Mouse over the tool buttons to see names or descriptions for the tools.
- Once you select a tool, information also displays above the drawing area.
- For details about drawing structures and using each of the tools, see the SciFinder Help files.

2. SciFinder provides you with options for presenting your results and further defining your search.

Click **Search**.

Explore Substances

Chemical Structure Molecular Formula Substance Identifier

Search

Click image to change structure or view detail

Search type: Exact Structure Substructure Similarity

Show precision analysis

Characteristic(s)

Single component Commercially available Included in reference(s)

Class(es)

Alloys Coordination compounds Incompletely defined Mixtures Polymers Organics, and others not listed

Studies

Analytical Biological Preparation Reactant or reagent

Tips:

- Change the search type (exact, substructure, or similarity) from what you already specified within the drawing editor.
- Specify whether you want to see a precision analysis (not available with stereo feature or similarity search).
- Select specific Characteristics, Classes, or Studies that you want to apply to your search.

3. Review your answers.

4. Answers from an Exact Search can include stereoisomers, isotopic variants, and multicomponent substances where the exact structure is one of the components.

Substances Get References Get Reactions Get Commercial Sources Combine Answer Sets

245 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Number of References

Answers per Page [15] 1 2 3 4 5 6 ... 17 View: [Icons]

1. Substance Detail 50-18-0

ClCCN(CCCl)P(=O)(O)O

C₇ H₁₅ Cl₂ N₂ O₂ P

2H-1,3,2-Oxazaphosphorin-2-amine, N, N-bis(2-chloroethyl)tetrahydro-, 2-oxide

~19,502 References Reactions Commercial Sources

2. Substance Detail 6055-19-2 (Component: 50-18-0)

ClCCN(CCCl)P(=O)(O)O.O

C₇ H₁₅ Cl₂ N₂ O₂ P · H₂ O

2H-1,3,2-Oxazaphosphorin-2-amine, N, N-bis(2-chloroethyl)tetrahydro-, 2-oxide, hydrate (1:1)

3. Substance Detail 60030-72-0

ClCCN(CCCl)P(=O)(O)O

C₇ H₁₅ Cl₂ N₂ O₂ P

Absolute stereochemistry.

2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide, (2R)-

~39 References Reactions

Tips:

- Use the **Sort by** list to sort your answers by Number of References or CAS Registry Number.
- Use the **View** icons to view substance answers in 1–4 columns.

5. Work with substances....

SciFinder allows you to work with substance answer sets in a variety of ways. For hints and tips, see the How To Guides for:

- Working with Substance Answer Sets: Overview
- Analyze Substance Answer Sets
- Refine Substance Answer Sets
- Obtain Commercial Sources
- View Properties
- Combine Answer Sets
- Print, Save, and Export Results

SciFinder also offers substructure and similarity searches. See the How To Guides for:

- Explore by Substructure
 - Explore by Structure Similarity
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