



toxplanet

TUTORIAL

Similar Compounds Searching

Similar Compounds is a powerful tool that fully automates the process of searching for chemical analogs. Using ToxPlanet's proprietary functionality, it allows for instant identification of structurally similar compounds. In this tutorial, we will look at how to search using Similar Compounds.

EXPERTIndex™ Search

Search Term

- Starts With
 Exact Match
 Contains

Submit

Clear

Full Text Search

MSDSonline® Advanced

TOXLINE® Special
AdvancedREACH Registrations
Advanced

Welcome to the ToxPlanet System

Our products have been designed to provide fast, easy, and intuitive access to a collection containing millions of documents covering over 1,000,000 unique substances. This page is intended to give you a quick overview of how our system works.

The ToxPlanet products can be searched using seven different Search Modes. Select from the left search panel to switch between Search Modes.

EXPERTIndex™ Search

Full Text Search

MSDSonline® Advanced

TOXLINE® Special Advanced

REACH Registrations Advanced

TSCATS Complete™ Advanced

ListEXPERT - List View

To search using Similar Compounds, begin by conducting an EXPERTIndex search. Start by clicking the **EXPERTIndex™ Search** button on the left side of the screen. This brings up a search box and several searching options (**Starts With**, **Exact Match**, and **Contains**). The “**Starts With**” radio button is enabled as it is the default setting.

EXPERTIndex™ Search

Search Term

- Starts With
- Exact Match
- Contains

Full Text Search

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EXPERTIndex™ Search

Full Text Search

MSDSonline® Advanced

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REACH Registrations Advanced

TSCATS *Complete*™ Advanced

ListEXPERT - List View

Enter the desired search term in the search box (for example, “*phenol*”), select a search option (for example, “**Exact Match**”), and click the **Submit** button to execute the search.

EXPERTIndex™ Search

Search Term

phenol

- Starts With
 Exact Match
 Contains

Submit

Clear

Full Text Search

MSDSonline® Advanced

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Advanced

Chemical Identity

ChemEXPERT™

ReproEXPERT™

ListEXPERT™

PoisonEXPERT™

REACH Registrations

C & L Inventory

DrugEXPERT™

TOXLINE® Special

ECIS

TSCATS Complete™

MSDSonline®

Similar Compounds

MyEXPERT™

Chemical Identity Search Results

Name of Substance

Phenol [USP:JAN]

CAS Registry Number

108-95-2

Molecular Formula

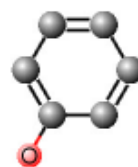
C6-H6-O

Other Registry Numbers

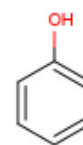
14534-23-7; 50356-25-7; 8002-07-1

SMILES

OC1=CC=CC=C1



Enlarge



Enlarge



NFPA 704



View



If there is an exact match in the EXPERTIndex, the system retrieves the Chemical Identity page for that substance.

EXPERTIndex™ Search

Search Term

phenol

- Starts With
 Exact Match
 Contains

Submit

Clear

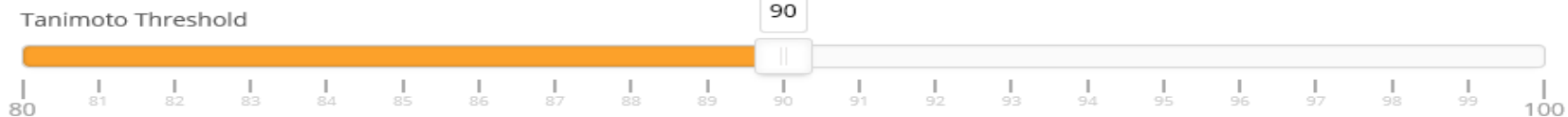
Full Text Search

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AdvancedREACH Registrations
AdvancedTSCATS
Complete™ Advanced

ListEXPERT - List View

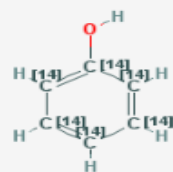
Chemical Identity ChemEXPERT™ ReproEXPERT™ ListEXPERT™ PoisonEXPERT™ REACH Registrations
C & L Inventory DrugEXPERT™ TOXLINE® Special ECIS TSCATS *Complete*™ MSDSonline® [Similar Compounds](#)
MyEXPERT™

Similar Compounds Search Results

Sort By: Chemical Name CAS Number % Similarity Ascending Descending
Page Size: 10 30 50 [About the results](#)

Prev 1 2 3 4 Next

showing 1 - 30 of 111

**Phenol-UL-14C**

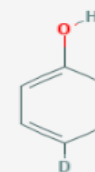
Similarity: 100%

CAS Registry Number: 53379-77-4

Molecular Formula: C₆H₆O

Molecular Weight: 106.066

SMILES: C1=CC=C(C=C1)O

InChI Key: ISWSIDIOOBJBQZ-
YROCTSJKSA-N**Phenol-4-d1**

Similarity: 100%

CAS Registry Number: 23951-03-3

Molecular Formula: C₆H₆O

Molecular Weight: 95.119

SMILES: C1=CC=C(C=C1)O

InChI Key: ISWSIDIOOBJBQZ-
MICDWDQJSA-N

Clicking the Similar Compounds tab returns a list of chemical compounds similar to the compound in your initial search. This display also provides additional information, including **Similarity %**, **CAS Registry Number**, **Molecular Formula**, **Molecular Weight**, **SMILES Notation**, **InChI Key**, as well as the number of compounds in the results list.

EXPERTIndex™ Search

Search Term

phenol

- Starts With
 Exact Match
 Contains

Submit

Clear

Full Text Search

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ListEXPERT - List View

Chemical Identity ChemEXPERT™ ReproEXPERT™ ListEXPERT™ PoisonEXPERT™ REACH Registrations
C & L Inventory DrugEXPERT™ TOXLINE® Special ECIS TSCATS *Complete™* MSDSonline® [Similar Compounds](#)
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Similar Compounds Search Results

Tanimoto Threshold

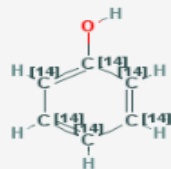


Sort By: Chemical Name CAS Number % Similarity Ascending Descending
Page Size: 10 30 50

[About the results](#)

Prev 1 2 3 4 Next

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Phenol-UL-14C

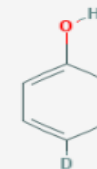
Similarity: 100%

CAS Registry Number: 53379-77-4

Molecular Formula: C6H6O

Molecular Weight: 106.066

SMILES: C1=CC=C(C=C1)O

InChi Key: ISWSIDIOOBJBQZ-
YROCTSJKSA-N

Phenol-4-d1

Similarity: 100%

CAS Registry Number: 23951-03-3

Molecular Formula: C6H6O

Molecular Weight: 95.119

SMILES: C1=CC=C(C=C1)O

InChi Key: ISWSIDIOOBJBQZ-
MICDWDJOJSA-N

You can navigate the results pages using the page number buttons, or by clicking “Prev” or “Next”.

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Search Term

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C & L Inventory DrugEXPERT™ TOXLINE® Special ECIS TSCATS *Complete*™ MSDSonline® [Similar Compounds](#)
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Similar Compounds Search Results

Tanimoto Threshold



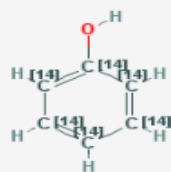
Sort By: Chemical Name CAS Number % Similarity Ascending Descending

Page Size: 10 30 50[About the results](#)

Prev 1 2 3 4 Next



showing 1 - 30 of 111



Phenol-UL-14C

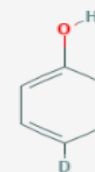
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You can also print current page results by clicking the purple PDF icon.

EXPERTIndex™ Search

Search Term

phenol

- Starts With
 Exact Match
 Contains

Submit

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Full Text Search

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AdvancedTSCATS
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ListEXPERT - List View

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C & L Inventory DrugEXPERT™ TOXLINE® Special ECIS TSCATS *Complete*™ MSDSonline® [Similar Compounds](#)
MyEXPERT™

Similar Compounds Search Results

Tanimoto Threshold

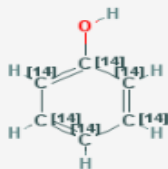


Sort By: Chemical Name CAS Number % Similarity Ascending Descending
Page Size: 10 30 50

[About the results](#)

Prev 1 2 3 4 Next

showing 1 - 30 of 111

**Phenol-UL-14C**

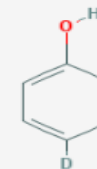
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Molecular Formula: C₆H₆O

Molecular Weight: 95.119

SMILES: C1=CC=C(C=C1)O

InChi Key: ISWSIDIOOBJBQZ-
MICDWDQJSA-N

By clicking on a compound in the results list, you will be able to view its Chemical Identity page (when available) and access all full-text documents available for that compound.

EXPERTIndex™ Search

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phenol

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Chemical Identity ChemEXPERT™ ReproEXPERT™ ListEXPERT™ PoisonEXPERT™ REACH Registrations
C & L Inventory DrugEXPERT™ TOXLINE® Special ECIS TSCATS *Complete*™ MSDSonline® [Similar Compounds](#)
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Similar Compounds Search Results

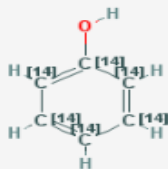
Tanimoto Threshold



Sort By: Chemical Name CAS Number % Similarity Ascending Descending
Page Size: 10 30 50 [About the results](#)

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Phenol-UL-14C

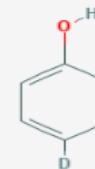
Similarity: 100%

CAS Registry Number: 53379-77-4

Molecular Formula: C6H6O

Molecular Weight: 106.066

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CAS Registry Number: 23951-03-3

Molecular Formula: C6H6O

Molecular Weight: 95.119

SMILES: C1=CC=C(C=C1)O

InChi Key: ISWSIDIOOBJBQZ-
MICDWDQJSA-N

Similar Compounds utilizes the Tanimoto coefficient, which mathematically calculates the degree of similarity between structures. By default, the level of similarity in the results is set at 90% (meaning the results shown are those with 90% structural similarity or greater). The level of similarity (and, in turn, the number of results) can be adjusted using the slide bar. You can also adjust the sort order and page size for the results using the corresponding radio buttons.

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Similar Compounds Search Results

Tanimoto Threshold



Sort By: Chemical Name CAS Number % Similarity Ascending Descending
Page Size: 10 30 50

[About the results](#)

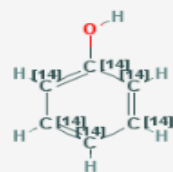
Prev

1

Next



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Phenol-UL-14C

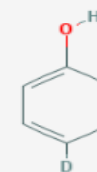
Similarity: 100%

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InChi Key: ISWSIDIOOJBQZ-
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Similarity: 100%

CAS Registry Number: 23951-03-3

Molecular Formula: C6H6O

Molecular Weight: 95.119

SMILES: C1=CC=C(C=C1)O

InChi Key: ISWSIDIOOJBQZ-
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Adjusting the threshold with the slide bar allows you to narrow or broaden your search requirements. In this example, changing the threshold from 90% to 100% displays only those compounds that are 100% similar to the chemical in the original search. There are fewer results (6 results at 100% vs. 111 results at 90%) due to increased specificity.



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www.toxplanet.com