



SciFinder<sup>®</sup>



# Alcance de SciFinder

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Química

Física

Biología

Ingeniería

Medicina

Agricultura

Materiales

Microbios

Farmacía

Textiles

Tecnología Nuclear

Geología

Y muchos más...

# ¿Qué es SciFinder?

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- Herramienta de CAS (división de ACS) desarrollada para que científicos la aprovechen, en las áreas de ciencias de la vida y ciencias de los materiales
- Interfaz de fácil uso
- Navegación intuitiva

<http://scifinder.cas.org>

# Bases de datos

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- Acceso a 6 bases de datos :
  - CAPLUS – Artículos, Patentes, Tesis, etc.
  - MEDLINE – Informaciones de la Salud
  - REGISTRY – Sustancias Químicas
  - CASREACT – Reacciones Químicas
  - CHEMCATS – Proveedores de Productos
  - CHEMLIST – Listas Reglamentarias

# Contenido

## CAPlus<sup>SM</sup>

- >31M bibliographic records
- >10K journals covered
- Patents from 61 patent offices
- Updated daily (~3K daily)
- Links to almost 300 publishers and 3 patent offices
- Literature back to early 1800s
- Cited articles from 1997 onward

## CAS REGISTRY<sup>SM</sup>

- 49M small molecules
- >61M sequences
- Updated daily (>12K daily)
- Substances reported comprehensively in literature back to 1957
- Includes nomenclature, spectra, and properties (experimental and predicted)

## CASREACT

- >18M single and multi-step reactions
- Extracted from patents and journal articles
- Updated weekly (~30K weekly)
- Reactions back to 1840
- Reaction conditions starting in 2003

## CHEMCATS

- >35M commercially available compounds
- >900 suppliers
- >1000 chemical catalogs
- Updated when new or revised catalogs are available
- Contact/ordering information including quantity and pricing (when available)

## CHEMLIST

- >248K inventoried / regulated substances
- >100 inventories & regulated lists from 1979 to present
- Updated weekly (~50 additions)
- Contains regulatory requirements for substances

## MEDLINE

- produced by the U.S. National Library of Medicine (NLM)
- > 18 million references
- Biomedical literature from more than 4,780 journals and 70 countries
- covering literature from 1950 to the present
- Updated 5 times per week

# Pantalla Principal - SciFinder On The Web

SciFinder®  
Welcome Ana Paula Hesse | Sign Out

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help  
KMP Alert Results | History  
SciPlanner | Preferences  
What's New

## Explore References

Research Topic

Examples:  
*The effect of antibiotic residues on dairy products*  
*Photocyanation of aromatic compounds*

Research Topic

Author Name  
Company Name  
Document Identifier  
Journal  
Patent  
Tags

Publication Year(s)   
Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Language(s)

<input type="checkbox"/> Chinese	<input type="checkbox"/> German	<input type="checkbox"/> Polish
<input type="checkbox"/> English	<input type="checkbox"/> Italian	<input type="checkbox"/> Russian
<input type="checkbox"/> French	<input type="checkbox"/> Japanese	<input type="checkbox"/> Spanish

Author Name     
Last \* First Middle

Saved Answer Sets   
No answer sets

Keep Me Posted Results   
No profiles exist

Página inicial con opciones de búsqueda, lista de las búsquedas guardadas y “keep me post”, etc.

# Características del SciFinder

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- La interfaz de búsqueda permite el uso de frases (límite hasta 5 palabras)
- Se pueden utilizar paréntesis para indicar los sinónimos de un concepto en particular.
- Se pueden utilizar “comillas” para encontrar conceptos exactos.
- Permite el uso de operadores Booleanos: OR, AND, WITH, NOT
- Emplea CAS RN en la búsqueda por tema
- SciFinder tiene un Thesaurus y un diccionario de sinónimos.

# SciFinder Smarts

Termino de Búsqueda	Terminos Asociados
Sinónimos incluyendo terminos controlados	- Paracetamol, Acetaminofen
Formas alternativas	- Freeze, froze, frozen, freezing - Waste water, wastewater - Antibacteriano, anti-bacteriano
Formas con plural irregular	- Woman, women - Ox, oxen - Mice, mouse, mousse - Half life, half-life, halflife, halflives, half live, half lives, halflive, halflives
Abreviaciones de CAS	- Oxidation, Oxidn
Escritura Americana y Britanica	- Synthesize, synthesise
<b>Reglas de trucagem</b> para recuperar palabras empezando por palabras de <b>tronco</b> comun	- Palabras terminadas en <b>-tion</b> con una raíz de por lo menos 5 letras son <b>truncadas</b> (depletion – deple?)- Palabras que contienen <b>-able, -ed, -ing</b> como sufijos son <b>truncadas</b> (solvable – solv?)- Palabras que contienen <b>-e</b> al final son <b>truncadas</b> (disease – diseas?)



# Búsqueda – Explore References

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Saved Answer Sets | Help  
KMP Alert Results | History  
SciPlanner | Preferences  
What's New

## Explore References

Research Topic  Search

Examples:  
*The effect of antibiotic residues on dairy products*  
*Photocyanation of aromatic compounds*

**Research Topic**

- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

Publication Year(s)

Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s)

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

Language(s)

<input type="checkbox"/> Chinese	<input type="checkbox"/> German	<input type="checkbox"/> Polish
<input type="checkbox"/> English	<input type="checkbox"/> Italian	<input type="checkbox"/> Russian
<input type="checkbox"/> French	<input type="checkbox"/> Japanese	<input type="checkbox"/> Spanish

Author Name

Last \* First Mid

**Ingresar con el término de búsqueda**

# Búsqueda – Explore References

**Publication Year(s)** ⓘ

Examples: 1995, 1995-1999, 1995-, -1995

**Document Type(s)** ⓘ

<input type="checkbox"/> Biography	<input type="checkbox"/> Dissertation	<input type="checkbox"/> Patent
<input type="checkbox"/> Book	<input type="checkbox"/> Editorial	<input type="checkbox"/> Preprint
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Historical	<input type="checkbox"/> Report
<input type="checkbox"/> Commentary	<input type="checkbox"/> Journal	<input type="checkbox"/> Review
<input type="checkbox"/> Conference	<input type="checkbox"/> Letter	

**Language(s)** ⓘ

<input type="checkbox"/> Chinese	<input type="checkbox"/> German	<input type="checkbox"/> Polish
<input type="checkbox"/> English	<input type="checkbox"/> Italian	<input type="checkbox"/> Russian
<input type="checkbox"/> French	<input type="checkbox"/> Japanese	<input type="checkbox"/> Spanish

**Author Name** ⓘ

<input type="text"/>	<input type="text"/>	<input type="text"/>
Last *	First	Middle

**Company Name** ⓘ

Examples:  
*Minnesota Mining and Manufacturing*  
*DuPont*

Campos para refinar ya en la página de búsqueda

# Resultados – Explore References



Explore References

Explore Substances

Explore Reactions

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Research Topic "acetaminophen and headache" ←

## Research Topic Candidates

5 Topics 0 Selected

Select All Deselect All

### Research Topic Candidates

References

<input type="checkbox"/>	2 references were found containing "acetaminophen and headache" as entered.	2
<input type="checkbox"/>	695 references were found containing both of the concepts "acetaminophen" and "headache". ←	695
<input type="checkbox"/>	113685 references were found containing either the concept "acetaminophen" or the concept "headache".	113685
<input type="checkbox"/>	37069 references were found containing the concept "acetaminophen".	37069
<input type="checkbox"/>	77311 references were found containing the concept "headache".	77311

Get References ←

Eligir los “candidatos” de su interés para llegar a la de resultados. Después, hacer clic en GET REFERENCES

# Resumen de Herramientas

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En la página de resultados, usted puede utilizar las siguientes herramientas:

- Analizar
- Categorizar
- Refinar
- Guardar respuestas (completa o parcial)
- Keep me Posted (completo o parcial)
- Obtener Referencias, Substancias, Reacciones, Citas, Fuente Comercial, Información Regulatoria, etc.

# Resumen del Documento

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Research Topic "acetaminophen and headache" > references (695)

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

695 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] 1 2 3 4 5 6 ... 35 Display: [icon]

1. Use of adenosine receptor agonists to modulate permeability of blood-brain barrier to treat central nervous system (CNS) disorders Full Text  
By Bynoe, Margaret S.  
From PCT Int. Appl. (2012), WO 2012037457 A1 20120322. | Language: English, Database: CAPLUS  
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From Faming Zhuanli Shenqing (2012), CN 102570004 A 20120517. | Language: Chinese, Database: CAPLUS  
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By Sawaddiruk, P.  
From Drugs of Today (2011), 47(10), 763-772.  
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Analysis Refine

Analyze by: [icon]

Author Name [dropdown]

Click bar to view only those references within the current answer set

Lipton R B	9
Diener H C	6
Faleck Herbert	6
Lipton Richard B	6
Manning Donald C	6
Silberstein Stephen D	6
Evers S	5
Haag Gunther	5

Hacer clic en el título del documento para llegar a la página del resumen y detalles, o en Full Text para acceder a la página del editor

# Resumen del Documento

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Research Topic "acetaminophen and headache" > references (695) > Buprenorphine 5, 10 and 20 µg/...

Reference Detail

Get Substances Get Reactions Get Cited Get Citing Get Full Text Send to SciPlanner

Link Save Print Export

Return

3. Buprenorphine 5, 10 and 20 µg/h transdermal patch: a review of its use in the management of chronic non-malignant pain

By: Plosker, Greg L.

This article reviews the pharmacol., therapeutic efficacy and tolerability profile of the 7-day lower-dose (5, 10 and 20 µg/h) buprenorphine transdermal patch (BuTrans, Norspan) in the management of chronic non-malignant pain, with a focus on European labeling for the drug. Buprenorphine is a semi-synthetic opioid analgesic that acts primarily as a partial agonist at the mu opioid receptor. The transdermal formulation provides continuous delivery of buprenorphine, resulting in relatively consistent plasma drug concns. throughout the 7-day dosing interval. The analgesic efficacy of transdermal buprenorphine in patients with osteoarthritis of the hip and/or knee has been demonstrated in several randomized controlled trials, which have shown the formulation to be equiv. to sublingual buprenorphine, noninferior to prolonged-release tramadol tablets, noninferior to codeine plus paracetamol (acetaminophen) combination tablets (when transdermal buprenorphine was used together with regularly scheduled oral paracetamol) and generally superior to a matching transdermal placebo patch. Transdermal buprenorphine was significantly more effective than placebo in reducing chronic low back pain of at least moderate severity in two randomized, double-blind, crossover trials. Other clin. trials, including a randomized, double-blind, maintenance-of-analgesia study, have also demonstrated the analgesic efficacy of transdermal buprenorphine in patients with chronic non-malignant pain of various causes. In general, serious adverse events with transdermal buprenorphine are similar to those for other opioid analgesics. Transdermal buprenorphine has a ceiling effect for respiratory depression, and the main risk is when it is combined with other CNS depressants. The most frequently reported adverse events with transdermal buprenorphine are headache, dizziness, somnolence, constipation, dry mouth, nausea, vomiting, pruritus, erythema, application site pruritus and application site reactions. Transdermal buprenorphine was better tolerated than sublingual buprenorphine in a 7-wk, randomized, double-blind trial in patients with osteoarthritis pain. Nevertheless, as with other opioids, persistence with transdermal buprenorphine therapy is difficult for many patients because of adverse events or other reasons. Thus, transdermal buprenorphine has generally demonstrated good efficacy and tolerability in clin. trials in chronic non-malignant pain, providing effective background analgesia as part of pain management strategies for patients with osteoarthritis, low back pain and other persistent pain syndromes of at least moderate severity. It also has favorable pharmacodynamic and pharmacokinetic properties, which have beneficial clin. implications, most notably the convenience of once-weekly administration and no need for dosage adjustments in the elderly or those with compromised renal function, making it an opioid of choice in these patients, and a useful therapeutic option overall in the management of chronic non-malignant pain.

Indexing

Pharmacology (Section1)

Quick Links

0 Tags, 0 Comments

Source

Drugs  
Volume71  
Issue18  
Pages2491-2509  
Journal  
2011  
CODEN:DRUGAY  
ISSN:0012-6667

Company/Organization

Adis, a Wolters Kluwer Business  
Auckland, N. Z.

Accession Number

2012:262941  
CAPLUS

Publisher

Wolters Kluwer Health

Language

Detalles del documento, informaciones bibliográficas, etc.

# CAS Full Text Options

**CAS**  
Full Text Options

[Logoff](#) | [Help](#)

**Buprenorphine 5, 10 and 20  $\mu$ g/h transdermal patch: a review of its use in the management of chronic non-malignant pain.**  
Drugs (2011), 71, (18), 2491-2509. Publisher: (Wolters Kluwer Health, ) CODEN:DRUGAY ISSN:0012-6667.

• [Email Reference](#)

Journal

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Publisher

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Hacer clic en Full Text para acceder el texto completo a través del CAS full text options®

# Analizar

The screenshot displays the SciFinder web interface. At the top, there are navigation options: "Explore References", "Explore Substances", and "Explore Reactions". A user is logged in as "Ana Paula Hesse". The main content area shows a list of 695 references for the topic "acetaminophen and headache". The first three references are visible, with the first one selected. The analysis sidebar on the right is highlighted with a red box, showing the "Analyze by:" dropdown menu set to "Author Name". Below this, a list of authors and their corresponding reference counts is shown.

References

695 References 0 Selected

Sort by: Accession Number

Answers per Page [20] 1 2 3 4 5 6 ... 35

Display: [List Icon]

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Analysis Refine

Analyze by: [Info](#)

Author Name

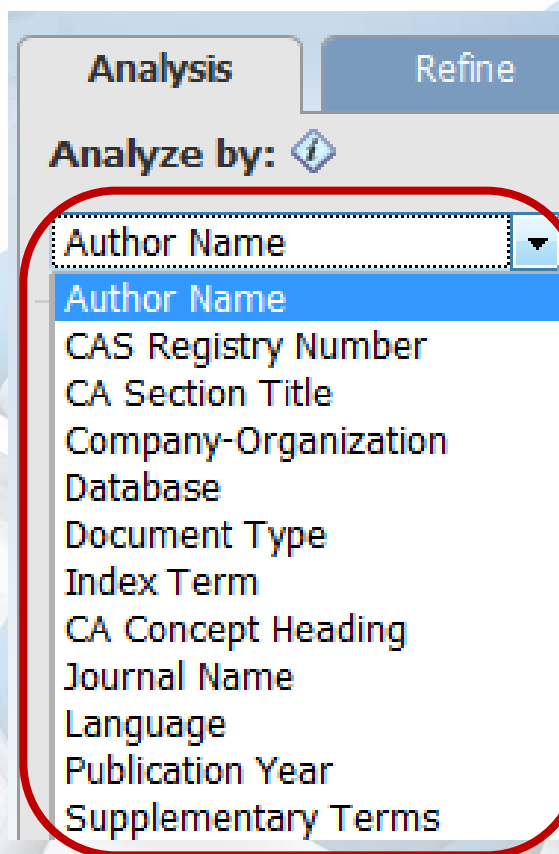
Click bar to view only those references within the current answer set

Lipton R B	9
Diener H C	6
Faleck Herbert	6
Lipton Richard B	6
Manning Donald C	6
Silberstein Stephen D	6
Evers S	5
Haag Gunther	5
Lewis Donald W	5

En la página de los resultados es posible analizar la lista por diferentes.



# Analizar



Analizar por nombre de autor, CAS RN, nombre de institución, tipo de documento, revista, idioma, año de publicación, etc.

# Refinar



Explore References

Explore Substances

Explore Reactions

Saved Answer Sets  
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Preferences  
What's New

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Research Topic "acetaminophen and headache" > references (695) > Buprenorphine 5, 10 and 20 µg/...

References Get Substances Get Reactions Get Related Tools Send to SciPlanner

695 References 0 Selected Save Print Export

Select All Deselect All Sort by: Accession Number

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Analysis Refine

Refine by:

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

[Input field]

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

En la página de resultados es posible refinar la lista por diferentes parámetros.

# Refinar

Analysis Refine

Refine by: ⓘ

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic

Refinar por t3pico de b3squeda, nombre de autor, nombre de instituci3n, tipo de documento, a3o de publicaci3n, idioma o base de datos.

# Búsqueda – Explore Substances

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Explore References | **Explore Substances** | Explore Reactions

Help | History | Preferences | What's New

Saved Answer Sets | KMP Alert Results | SciPlanner

## Explore Substances

Chemical Structure | Chemical Structure | Search

- Chemical Structure
- Markush
- Molecular Formula
- Property **NEW**
- Substance Identifier

Click to Edit

Characteristic(s)

- Single component
- Commercially available
- Included in reference(s)

Class(es)

- Alloys
- Coordination compounds
- Incomplete
- Mixtures
- Polymers
- Gases and other listed

Studies

- Analytic
- Biologic

Heat transfer process unam REACTION

View All

Import

Keep Me Posted Results

campos de petróleo No results

View All

Para búsqueda de sustancias utilizando fórmula estructural, hacer clic en la imagen para activar el plug-in de dibujo.

SciFinder®

# Búsqueda – Explore Substances

The screenshot displays the 'Structure Editor' window. The central workspace shows a naphthalen-1-ol molecule (SMILES: Oc1ccc2ccccc12), which is highlighted with a red rounded rectangle. To the left, a vertical toolbar is also highlighted with a red rounded rectangle, containing various drawing tools such as 'Atom', 'Short', and 'Bond'. At the top right, a 'Shortcut Keys' button is highlighted with a red rounded rectangle. On the right side, the 'Drawing Editor' panel is highlighted with a red rounded rectangle, featuring radio buttons for 'Structure' (selected), 'Reaction', and 'Markush'. Below it, the 'Get substances that match your query using:' panel is highlighted with a red rounded rectangle, showing radio buttons for 'Exact search' (selected), 'Substructure search', and 'Similarity search', along with 'OK' and 'Cancelar' buttons. The bottom status bar includes a text input field with 'OH', a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a 'Scale 100' control.

Plug-in para dibujo de la fórmula estructural

# Búsqueda – Explore Substances

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Explore References | Explore Substances | Explore Reactions

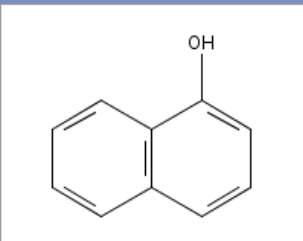
Research Topic "acetaminophen and headache" > references (644) > Methyloxanthines and pain

## Explore Substances

**Chemical Structure** | Chemical Structure

Markush  
Molecular Formula  
Substance Identifier

**Search**



Click image to change structure or view detail

Search type:  Exact Structure  
 Substructure  
 Similarity

Show precision analysis

**Saved Answer Sets**

- Ureia\_Hexion
- Omepraz\_patente
- 1-Naphtol\_patentes
- Omeprazole
- omeprazole
- Autosaved Reference Set

View All

**Import**

**Keep Me Posted Results**

No profiles exist

**My Connections**

No invitations to connect  
No outstanding sent invitations  
You have 1 connection

La fórmula estructural el término de búsqueda.  
Mas abajo hay algunas herramientas de refino.

# Búsqueda – Explore Substances

Chemical Structure

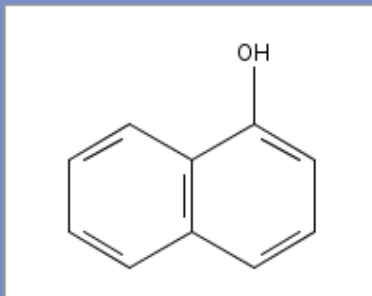
Chemical Structure ⓘ

Search

Markush

Molecular Formula

Substance Identifier



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

Opciones para refinar y direccionar la lista de resultados.

# Resultados – Explore Substances



Explore References

Explore Substances

Explore Reactions

Saved Answer Sets

Help

KMP Alert Results

History

SciPlanner

Preferences

What's New

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Chemical Structure exact with limiters > substances (54) > 90-15-3

Substances Get References Get Reactions Tools Send to SciPlanner

54 Substances 0 Selected

Save Print Export

Select All Deselect All Sort by: Relevance (New)

Answers per Page [15] 1 2 3 4

View: [Icons]

Analysis Refine

Analyze by:

Substance Role

Click bar to view only those substances within the current answer set

Properties 33

Formation, Nonpreparative 29

Reactant or Reagent 26

Preparation 25

Process 24

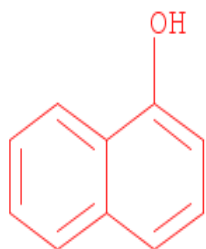
Uses 7

Biological Study 6

Analytical Study 5

1. Substance Detail 90-15-3

~11399

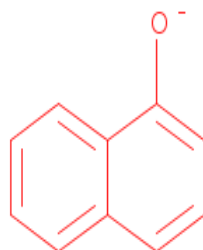


C<sub>10</sub> H<sub>8</sub> O  
1-Naphthalenol

Spectra  
Experimental Properties

2. Substance Detail 17545-30-1

~82

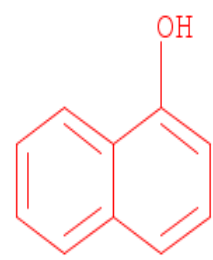


C<sub>10</sub> H<sub>7</sub> O  
1-Naphthalenol, ion(1-)

3. Substance Detail 26716-77-8

~86

90-15-3  
C<sub>10</sub> H<sub>8</sub> O



(C<sub>10</sub> H<sub>8</sub> O)<sub>x</sub>  
1-Naphthalenol, homocopolymer

4. Substance Detail 33490-96-9

~36



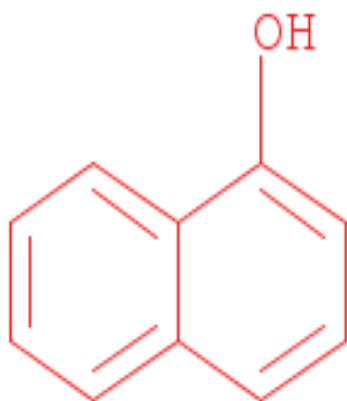
5. Substance Detail 72773-99-0

Página de resultados con herramientas para analizar y refinar.



# Resultados – Explore Substances

1. Substance Detail  
90-15-3



C<sub>10</sub> H<sub>8</sub> O  
1-Naphthalenol



Spectra  
Experimental Properties

Desde los resultados es posible acceder:

1. Detalles de la Substancia
2. Documentos sobre a Substancia
3. Reacciones de la substancia
4. Proveedores
5. Información Regulatoría
6. Espectros y Propiedades Experimentales

# Detalles de la Substancia

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert Chemical Structure exact with limiters > substances (54) > 90-15-3

## Substance Detail



Get References



Get Reactions



Get Commercial Sources



Get Regulatory Info



Send to SciPlanner

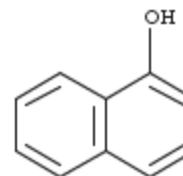
**CAS Registry Number:** 90-15-3

C<sub>10</sub> H<sub>8</sub> O

1-Naphthalenol

1-Naphthol (8CI); 1-Hydroxynaphthalene; 1-Naphthyl alcohol; BASF Ursol ERN; C.I. 76605; C.I. Oxidation Base 33; Durafur Developer D; Fouramine ERN; Fournine 99; Fournine ERN; Furro ER; NSC 9586; Nako TRB; Naphthol-1; Naphthyl-1-ol; Tertral ERN; Ursol ERN; Zoba ERN;  $\alpha$ -Hydroxynaphthalene;  $\alpha$ -Naphthol;  $\alpha$ -Naphthyl alcohol

**Deleted CAS Registry Numbers:** 50356-21-3



~11,399 References

**Document Types:** Conference, Dissertation, Journal, Patent, Preprint, Report

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study				
Combinatorial Synthesis				
Formation, Non				
Miscellaneous				
Occurrence				

Detalles de la sustancia tal como nombres, fórmulas, propiedades experimentales y estimadas, etc

# Detalles de la Substancia

Predicted Properties: [Biological](#) [Chemical](#) [Density](#) [Lipinski and Related](#) [Spectra](#) [Structure-related](#) [Thermal](#)

Biological Properties	Value	Condition	Note
Bioconcentration Factor	69.3	pH 1 Temp: 25 °C	(85)
Bioconcentration Factor	69.3	pH 2 Temp: 25 °C	(85)
Bioconcentration Factor	69.3	pH 3 Temp: 25 °C	(85)
Bioconcentration Factor	69.3	pH 4 Temp: 25 °C	(85)
Bioconcentration Factor	69.3	pH 5 Temp: 25 °C	(85)
Bioconcentration Factor	69.2	pH 6 Temp: 25 °C	(85)
Bioconcentration Factor	69.0	pH 7 Temp: 25 °C	(85)
Bioconcentration Factor	66.6	pH 8 Temp: 25 °C	(85)
Bioconcentration Factor	49.6	pH 9 Temp: 25 °C	(85)
Bioconcentration Factor	13.9	pH 10 Temp: 25 °C	(85)

Chemical Properties	Value	Condition	Note
Koc	723	pH 1 Temp: 25 °C	(85)
Koc	723	pH 2 Temp: 25 °C	(85)
Koc	723	pH 3 Temp: 25 °C	(85)
Koc	723	pH 4 Temp: 25 °C	(85)
Koc	723	pH 5 Temp: 25 °C	(85)
Koc	723	pH 6 Temp: 25 °C	(85)
Koc	720	pH 7 Temp: 25 °C	(85)
Koc	695	pH 8 Temp: 25 °C	(85)
Koc	517	pH 9 Temp: 25 °C	(85)
Koc	146	pH 10 Temp: 25 °C	(85)
logD	2.72	pH 1 Temp: 25 °C	(85)
logD	2.72	pH 2 Temp: 25 °C	(85)
logD	2.72	pH 3 Temp: 25 °C	(85)

Propiedades Estimadas

# Detalles de la Substancia



Experimental Properties: [Biological](#) [Chemical](#) [Density](#) [Electrical](#) [Lipinski and Related](#) [Optical and Scattering](#) [Spectra](#) [Structure-related](#)  
[Thermal](#)

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text		(2) CAS
LC50	See full text	1 of 3	(29) CAS
Median Lethal Dose(LD50)	2400 mg/kg	Organism: rat Route: oral	(32) CAS
Minimum Inhibitory Concentration	See full text		(76) CAS

Chemical Properties	Value	Condition	Note
Acid/Base Dissociation Constant (Ka/Kb)	See full text	1 of 3	(1) CAS
Dissociation Constant	See full text		(21) CAS
logP	See full text	1 of 2	(30) CAS
Molecular Electric Dipole Moment	See full text		(77) CAS
Partition Coefficient	See full text	1 of 12	(78) CAS
Potential of Electrode Reaction	See full text	1 of 4	(25) CAS
Solubility	See full text		(80) CAS

Density Properties	Value	Condition	Note
Density	1.22 g/cm3	Temp: 4 °C	(4) CAS
Density	1.0954 g/cm3	Temp: 98.7 °C	(5) NLM

Electrical Properties	Value	Condition	Note
Dielectric Constant	See full text		(20) CAS

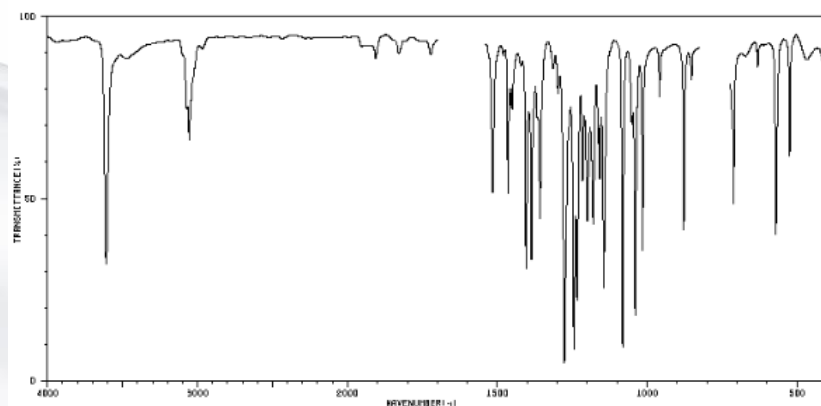
Lipinski and Related Properties	Value	Condition	Note
logP	See full text	1 of 2	(30) CAS

Optical and Scattering Properties	Value	Condition	Note
Refractive Index	1.9224		
Refractive Index	1.6224	Waven: 369.3 nm; Temp: 99 °C	(3) NLM
Refractive Index	1.6110	Waven: 590.3 nm; Temp: 30 °C	(6) CAS

Propiedades Experimentales

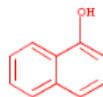
# Espectros RMN, IR, etc

IR Absorption Spectrum

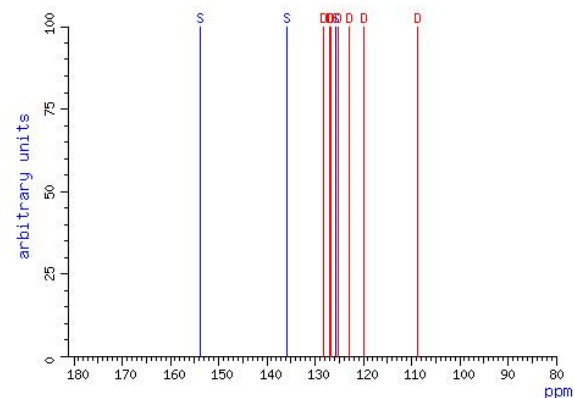


CAS Registry Number: 90-15-3

C<sub>10</sub>H<sub>8</sub>O  
1-Naphthalenol

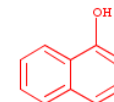


Carbon-13 NMR Spectrum



CAS Registry Number: 90-15-3

C<sub>10</sub>H<sub>8</sub>O  
1-Naphthalenol



Acceso a diferentes tipos de espectros de la sustancia.

# Reacciones

SciFinder®

Welcome Edison Penachin | Sign Out

Create Keep Me Posted "Research Topic "acetaminophen and headache" > references (644)

Explore References Explore Substances Explore Reactions

Saved Answer Sets Help  
Keep Me Posted Results History  
My Connections Preferences

Explore Reactions

Reaction Structure Reaction Structure

Click to Edit

Solvent(s)

Non-participating Functional Group(s)

Number of Steps   
Examples: 1, 1 - 3, 1 -, - 3

Classification(s)  Biotransformation  Electrochemical  Radiochemical

Saved Answer Sets

Ureia\_Hexion  
Omepraz\_patente  
1-Naphtol\_patentes  
Omeprazole  
omeprazole  
Autosaved Reference Set

View All

Keep Me Posted Results

No profiles exist

My Connections

No invitations to connect  
No outstanding sent invitations  
You have 1 connection

Para búsqueda de reacciones, hacer clic en la imagen para activar el plug-in de dibujo.

# Reacciones

The screenshot displays the Reaction Editor window. The main workspace shows a chemical reaction: aniline (a benzene ring with an NH<sub>2</sub> group) is converted to nitrobenzene (a benzene ring with an NO<sub>2</sub> group). The reactant is labeled "reactant/reagent" and the product is labeled "product".

On the left side, a vertical toolbar is highlighted with a red box. It contains various drawing tools such as "Atom", "Short", "-X", "=R", "[ ]", "1-4", "Cl", "W", "R", "K", "A", "B", "alchc", "ketor", and "alder".

At the top right, a "Drawing Editor" panel is highlighted with a red box. It contains three radio buttons: "Structure", "Reaction" (which is selected), and "Markush".

At the bottom right, another panel is highlighted with a red box. It is titled "Get reactions where the structure(s) are:" and contains two radio buttons: "Variable only at the specified positions" (which is selected) and "Substructures of more complex structures".

At the bottom of the window, there is a search bar containing "NO2", a list of elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a "Scale" field set to 100. Below this are several icons for drawing rings and bonds.

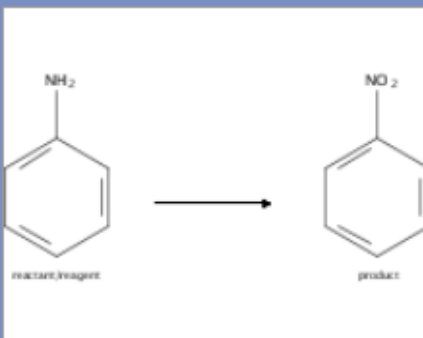
Dibujar la reacción

# Reacciones

## Explore Reactions

Reaction Structure

Reaction Structure ⓘ



Click image to change structure or view detail

Search

Search type: ⓘ  Allow variability only as specified  
 Substructure

Solvent(s) ⓘ

≡ Select Solvents

Non-participating  
Functional Group(s) ⓘ

≡ Select Groups

Number of Steps ⓘ

1-2

Examples: 1, 1 - 3, 1 -, - 3

El término de búsqueda es la reacción. Es posible utilizar filtros.



# Reacciones - Resultados

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Add KMP Alert Reaction Structure structure variable only at spe... with limiters > reactions (61)

Reactions

Get References

Tools

Send to SciPlanner

Analysis

Refine

Analyze by:

Catalyst

Click bar to view only those reactions within the current answer set

RuCl<sub>3</sub> 9

MeN<sup>+</sup>((CH<sub>2</sub>)<sub>7</sub>Me)<sub>3</sub> • Cl<sup>-</sup> 7

1034805-97-4 2

1343-93-7 2

851956-06-4 2

851956-08-6 2

t-BuOOH 2

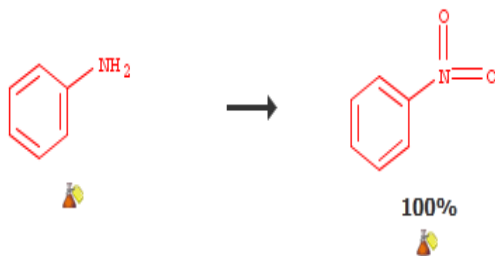
61 Reactions 0 Selected

Select All Deselect All Sort by: Relevance

Answers per Page [15] 1 2 3 4 5

Display:

1. View Reaction Detail Link Similar Reactions  
Single Step Hover over any structure for more options.



Overview

Steps/Stages

Notes

1.1 R:H<sub>2</sub>O<sub>2</sub>, C:1034805-97-4, C:MeN<sup>+</sup>((CH<sub>2</sub>)<sub>7</sub>Me)<sub>3</sub> • Cl<sup>-</sup>, S:H<sub>2</sub>O, S:t-BuOMe<sub>3</sub>, 7 h, 60°C

green chemistry - catalyst, green chemistry - solvent, selective oxidation, multiphase

En la página de resultados, la lista de reacciones que atienden a los criterios de la búsqueda y herramientas para analizar o refinar.

# Herramientas – Páginas de Resultados

Welcome Ana Paula Hesse | Sign Out

Add KMP Alert

Research Topic "acetaminophen and headache" > references (695)

References



Get Substances



Get Reactions



Get Related



Tools



Send to SciFinder

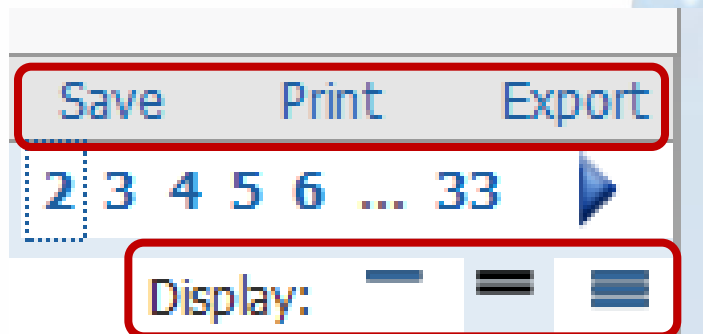
695 References 0 Selected

Select All Deselect All Sort by Accession Number

En las páginas de resultados hay diferentes herramientas tales como Keep Me Posted, Get Substances, Get Reactions, Artículos Citados, Artículos Citantes, Acceso a Texto Completo, Combinar lista de resultados, etc

# Herramientas – Páginas de Resultados

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En las páginas de resultados es possible Guardar, Imprimir o Exportar la lista completa de resultados, o aquellos seleccionados. Tambien es posible definir cómo mostrar la lista.

**Alerta:** El limite de downloads por sesión es 5.000 títulos.

# SciPlanner

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O SciPlanner es una nueva herramienta disponible en el SciFinder que permite crear y administrar proyectos de síntesis orgánica, asociando sustancias, reacciones y bibliografías.

Un video esta disponible con un ejemplo de su utilización, en el link:

<http://www.youtube.com/watch?v=T73Ojm3-3Ts>

<http://www.cas.org/etrain/scifinder/sciplanner.html>

# Herramientas en la Web

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<http://www.cas.org/support/scifi/index.html>

# Contacto

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Mónica Arriagada Delgado

[monica.arriagada@itmsgroup.net](mailto:monica.arriagada@itmsgroup.net)