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Chemical Sciences

# BÚSQUEDA SIMPLE DE UN COMPUESTO

About

More Searches

Web APIs

Help

eg. Pyridine

Search

Search



Search

Simple Structure Advanced More searches...

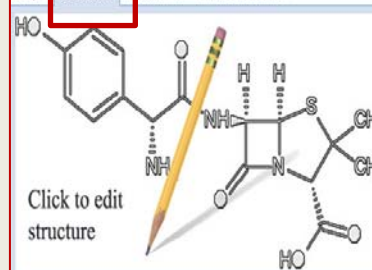
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

Options

 Search

Search

Simple Structure Advanced More searches...




- Exact
- Substructure
- Similarity

Search Options

- Exact Match
- All Tautomers
- Same Skeleton (Including H)
- Same Skeleton (Excluding H)
- All Isomers

Options

 Search

Search Hits Limit: 100

Simple Structure **Advanced** More searches...

- Search by Structure ?
- Search by Identifier ?
- Search by Elements ?
- Search by Properties ?
- Search by Calculated Properties ?
- Search by Data Source, Data Source Type or Focused Library ?
- Search by LASSO Similarity ?

Options

 Search

Search Hits Limit: 100

Search

Simple Structure Advanced More searches...

- Search by Structure ?
- Search by Identifier ?
- Search by Elements ?
- Search by Properties ?
- Search by Calculated Properties ?
- Search by Data Source, Data Source Type or Focused Library ?
- Search by LASSO Similarity ?

Options

 Search

Search Hits Limit: 100

BÚSQUEDA

SIMPLE

RSC SyntheticPages Login Register

 **ChemSpider**  
The free chemical database

About More Searches Web APIs Help

**Búsqueda simple por "colesterol"**

Search

Simple Structure Advanced More searches...


cholestel  
Cholesteryl  
cholesteryl linoleate  
Cholesteryl linolenate  
Cholesteryl palmitoleate  
cholestene-3,24,27-triol  
Cholestenediol  
cholestenetriol  
Cholestenone  
Cholesteryl butyrate  
Cholesterin  
Cholesterin acetate  
Cholesterin ethyl ether  
Cholesterin methyl ether  
**Cholesterol**  
Cholesterol 3beta-oleate  
cholesterol 3-sulfate  
Cholesterol 3-tosylate  
Cholesterol Acetate

Search Hits Limit: 100

Waters  
THE SCIENCE OF WHAT'S POSSIBLE™

YOU COULD ADVERTISE

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 **ChemSpider**  
The free chemical database

About More Searches Web APIs Help

eg. Pyridine Search

Search

Simple Structure Advanced More searches...

Cholesterol  
*Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID*

Options

Search

Search Hits Limit: 100

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[EMPOWER]  
LEARN MORE

Search term: Cholesterol (Found by approved synonym)

### Cholesterol

ChemSpider ID: 5775  
Molecular Formula: C<sub>27</sub>H<sub>46</sub>O  
Monoisotopic mass: 386.354858 Da

Systematic name  
(3β)-Cholest-5-en-3-ol

SMILES and InChI

2D 3D Save Zoom  
- 8 of 8 defined stereocentres

Want to comment on this record?  
Leave Feedback

Posibilidad de realizar comentarios, correcciones, información, etc. sobre este compuesto.

Datos básicos de la estructura (fórmula, masa, nombre), descargar, zoom, vista en 3D, códigos.

SMILES:  
C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C [Copy](#)

Std. InChI:  
InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(20)13-15-26(20,1)25(22)14-16-27(23,24)5/h9,18-19,21-25,28H,6-8,10-,23-,24+,25+,26+,27-/m1/s1 [Copy](#)

AQBDFSA-N [Copy](#)

#### Names and Identifiers

Names and Synonyms Database ID(s)

Validated by Experts, Validated by Users, Non-Validated by Users, Redirected by Users, Redirect Approved by Experts [Edit](#)

(-)-Cholesterol  
(3b)-cholest-5-en-3-ol  
(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-[[...]]  
(3S,8S,9S,10R,13R,14S,17R)-10,13-Diméthyl-17-[[...]]  
[French]  
(3β)-cholest-5-en-3-ol [ACD/IUPAC Name]  
(3β)-Cholest-5-én-3-ol [French]  
3b-Hydroxy-5-cholestene  
3β-Hydroxycholest-5-ene  
5:6-Cholesten-3b-ol  
5:6-Cholesten-3β-ol  
[More...](#)

Otros nombres e IDs relacionadas con la estructura.

Búsquedas a medida para realizar búsquedas avanzadas tanto en ChemSpider como en otros sitios externos a la base de datos.

#### ChemSpider Searches

Search ChemSpider for:

- Records with the same molecular formula
- Compounds with the same skeleton
- Use this molecule in a structure search

Search external sites for this structure:

- Search Google Scholar (by synonym)
- Search Google for exact structure
- Search Google for structures with same skeleton

Print

**Properties** ? Print

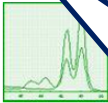
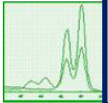
Experimental data | Predicted - ACD/Labs | Predicted - EPISuite | Predicted - ChemAxon

data supplied by datasources and users.

- Experimental Physchem Properties**
  - Melting Point: 149 ? 🔗
  - Melting Point: 147-150? ? 🔗
  - Melting Point: 147-150? ? 🔗
  - Melting Point: 147-150 ? 🔗
  - Melting Point: 148 - 150 C ? 🔗
  - Boiling Point: 360? ? 🔗
  - Boiling Point: 360? ? 🔗
  - Boiling Point: 360 ? 🔗
  - Boiling Point: 360 C ? 🔗
  - Flash Point: White powder ? 🔗
  - Flash Point: White powder ? 🔗
  - Specific Gravity: 1.067 ? 🔗
  - Specific Gravity: 1.067 ? 🔗
  - Optical Rotation: -36 (c=2 in dioxane) ? 🔗
  - Optical Rotation: -36 (c=2 in dioxane) ? 🔗
  - Optical Rotation: -36 (c=2 in dioxane) ? 🔗
- Miscellaneous**
  - Appearance: Cholesterol, 95% ? 🔗
  - Appearance: Cholesterol, 95% ? 🔗
  - Appearance: white crystalline powder ? 🔗
  - Stability: Stable. Combustible. Incompatible with strong oxidizing agents. ? 🔗
  - Safety: WARNING: Not for human consumption, may irritate skin & eyes. ? 🔗
  - Safety: WARNING: Not for human consumption, may irritate skin & eyes. ? 🔗
  - Safety: WARNING: Not sold for human treatment, trials or use ? 🔗
  - Safety: Apparently of low toxicity. Use normal good housekeeping measures. ? 🔗

Información sobre datos de propiedades tanto teóricas como experimentales.

**Spectra** ? Add

- Type:** CNMR  
**Approved:** Yes  
**Submitted by:** ChemSpiderman
-  Download
- Type:** HNMR  
**Approved:** Yes  
**Submitted by:** ChemSpiderman
-  Download
- Type:** HNMR  
**Associated Hyperlink:** <http://rainier.chem.plu.edu/nutsform.html>  
**Comments:** These data are obtained from the Pacific Lutheran University FTNMR FID Archive

Espectros interactivos (NMR, MS, IR, UV-Vis) que pueden estar asociados a publicaciones o a webs de grupos de investigación

**Articles** ? Print

Links & Reference ? RSC Journals RSC Books PubMed MeSH Literature Google Books

- H.-S. Shieh and C. E. Nordman. Cholesterol hemimethanol solvate, *Acta Cryst.* (2002). *E58*, o79-o80Å Å Å Å  
[DOI: 10.1107/S1600536801020487]
- Bosco et al.. Elevated levels of oxidized cholesterol metabolites in Lewy body disease brains accelerate alpha-synuclein fibrilization, *Nature Chemical Biology*, 2006  
[DOI: 10.1038/nchembio782]
- Polozov et al.. Progressive Ordering with Decreasing Temperature of the Phospholipids of Influenza Virus, *Nature Chemical Biology*, 2008  
[DOI: 10.1038/nchembio.77]
- Meloni et al.. Metal swap between Zn7-metallothionein-3 and beta Cu protects against amyloid-beta toxicity, *Nature Chemical Biology*, 2008  
[DOI: 10.1038/nchembio.89]
- Gerlach et al.. HIV-1 Nef membrane association depends on membrane lipid composition and sequence, *Nature Chemical Biology*, 2009  
[DOI: 10.1038/nchembio.268]
- Tobias Kind, Martin Scholz, Oliver Fiehn. How Large is the Metabolome of a Species? *PLoS ONE* 4(5): e5440  
[DOI: 10.1371/journal.pone.0005440]  
Calculating the metabolome size of species by lack of annotated genes. Hence, metabolomes databases could be queried to compile target list knowledge base of metabolites.
- Mével Mathieu. Novel neutral imidazole-lipophospholipids, *PLoS ONE* 4(5): e5440  
[DOI: 10.1039/b805226c]
- Aparicio Jesús F.. Microbial cholesterol oxidases: bioconversion enzymes or signal proteins?, *Molecular BioSystems*, 2008  
[DOI: 10.1039/b717500k]
- Numata Munenori. Creation of polynucleotide-assisted molecular assemblies in organic solvents: general strategy toward the creation of artificial DNA-like nanoarchitectures, *Organic & Biomolecular Chemistry*, 2008  
[DOI: 10.1039/b713354e]

**Publicaciones relacionadas con el compuesto de búsquedas, en este caso, colesterol.**

**Chemical Vendors** ? Print

Data Source	External ID(s)
R&D Chemicals <span>?</span>	3551
Aronis <span>?</span>	BBC/344
Trylead Chemical <span>?</span>	TL8003721
Sigma-Aldrich <span>?</span>	S5442_SIGMA, C3292_SIGMA, C1231_SIGMA, C3137_SIGMA, C3045_SIGMA, C8503_SIGMA, C8667_SIGMA, 47127U_SUPELCO, 26740_FLUKA, 26732_FLUKA
Alfa Aesar <span>?</span>	A11470
Timtec <span>?</span>	SBB058670
Extrasynthese <span>?</span>	3551, 3506
Pharmten <span>?</span>	S-PTN26633
Molport <span>?</span>	MolPort-002-506-911
Zerenex Molecular <span>?</span>	ZXN000114, ZX-AS001340
Research Organics <span>?</span>	RES1387C-A102X, RES1387C-A103X
Santa Cruz Biotechnology <span>?</span>	sc-202539
Tokyo Chemical Industry Ltd <span>?</span>	C0318
Finetech Industry <span>?</span>	FT-57-88-5
InterBioScreen <span>?</span>	BB_NC-0135, STOCK1N-54186
Fluorochem <span>?</span>	121530
Paragos <span>?</span>	490008
ABI Chemicals, GmbH <span>?</span>	AC1Q1PAZ

**Información sobre si el compuesto está disponible comercialmente y posibilidad de conectar con la web del vendedor.**

**Data Sources** Print Filter

[Chemical Vendors](#)
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[Data Aggregators](#)
[Safety Data](#)
[All Data Sources](#)

Data Source	External ID(s)
R&D Chemicals	3551
Aronis	BBC/344
Trylead Chemical	TL8003721
Sigma-Aldrich	S5442_SIGMA, C32947127U_SUPELCO, A11470
Alfa Aesar	
Timtec	SBB058670
Extrasynthese	3551, 3506
Pharmten	S-PTN26633
Molport	MolPort-002-506-911
	ZYN000114_ZY_AS001340

Enlaces con todas las fuentes que han contribuido a la información sobre este registro, agrupadas por materias.

**Wikipedia Article(s)** Print License

**Cholesterol**, from the Greek *chole-* (bile) and *stereos* (solid) followed by the chemical suffix *-ol* for an alcohol, is an organic chemical substance classified as a waxy steroid of fat. It is an important structural component of mammalian cell membranes and is required to establish proper membrane permeability and fluidity. In addition, it is a precursor in the hormonal systems of the body for the manufacture of bile acids, steroid hormones, and vitamin D. It is synthesized by animals; in vertebrates it is formed predominantly in the liver. Small amounts are also synthesized by plants and fungi. It is almost completely absent among prokaryotes, i.e. bacteria and archaea. High levels of cholesterol in the blood have been linked to damage to arteries.

[Read full article at Wikipedia...](#)  
[Edit article at Wikipedia...](#)

**Patents** Print

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[USPTO Applications](#)
[European Granted](#)
[European Applications](#)
[WO/PCT](#)
[Japanese Abstracts](#)

[Mammalian pancreatic cholesterol esterase](#)

Patente estadounidense 5981 MAMMALIAN PANCREATIC CHOLESTEROL ESTERASE now US Pat. No. 5,981,000

of application Ser. No. 08/461881, filed Jun. 5, 1995.

[Mammalian pancreatic cholesterol esterase](#)

Enlaces a los artículos de Wikipedia

Visión general sobre patentes

**RSC Databases**

- Description
- Medical Subject Headings Classification
- Pharmacological Links


Resto de información disponible, que podemos extender o comprimir situándonos sobre la flecha.



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# BÚSQUEDA POR ESTRUCTURA (EDITOR DE DIBUJO)



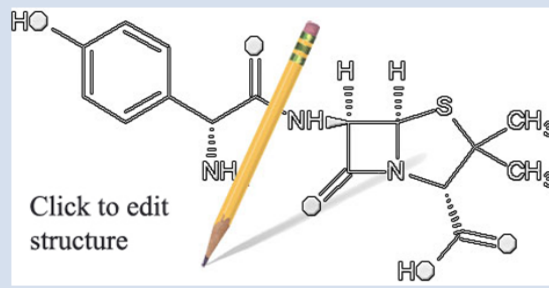

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About More Searches Web APIs

eg. Pyridine

**Búsqueda por estructura**

Search Simple **Structure** Advanced More searches...



Click to edit structure

Options


Exact  
 Substructure  
 Similarity

**Search Options**

Exact Match  
 All Tautomers  
 Same Skeleton (Including H)  
 Same Skeleton (Excluding H)  
 All Isomers

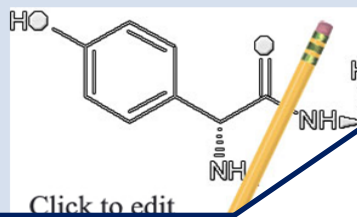
**Opciones de búsqueda**

Search Hits Limit: 100



About More Searches Web APIs

Search Simple **Structure** Advanced More searches...





Click to edit structure

Options

**ChemSpider | Input Chemical Structure - Windows Internet Explorer**

Draw structure Load structure Convert identifier to structure





Accelrys JDraw  Elemental  ACD/Labs SDA  Ketcher  JME  JChemPaint

Internet 100%

Búsqueda por estructura

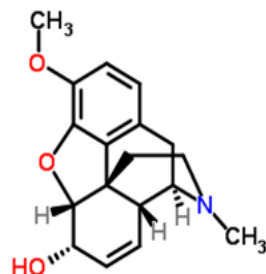
Opciones de búsqueda

Otras opciones de editar la estructura sin dibujarla

Se puede elegir entre distintos editores de dibujo

Con las distintas herramientas del editor dibujamos la molécula, la codeína.

Search term: SEARCH\_BY\_MOLECULE Exact (Finished)



2D 3D Save Zoom

- 5 of 5 defined stereocentres

## Codeine

ChemSpider ID: **4447447**

Molecular Formula: C<sub>18</sub>H<sub>21</sub>NO<sub>3</sub>

Monoisotopic mass: 299.15213 Da

Systematic name

(5 $\alpha$ ,6 $\alpha$ )-3-Methoxy-17-methyl-7,8-didehydro-4,5-epoxymorphinan-6-ol

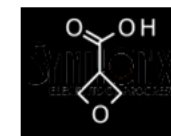
SMILES and InChIs

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### Names and Identifiers

Print

Names and Synonyms Database ID(s)

Validated by Experts, Validated by Users, Non-Validated, Removed by Users, Redirected by Users, Redirect Approved by Experts

Edit

Codeine [Wiki] [USP] [INN] [BAN]

(-)-codeine

(1S,5R,13R,14S,17R)-10-Methoxy-4-methyl-12-oxa-4-azapentacyclo[9.6.1.0<sup>1,13</sup>.0<sup>5,17</sup>.0<sup>7,18</sup>]octadeca-7(18),8,10,15-tetraen-14-ol

(1S,5R,13R,14S,17R)-10-méthoxy-4-méthyl-12-oxa-4-azapentacyclo[9.6.1.0<sup>1,13</sup>.0<sup>5,17</sup>.0<sup>7,18</sup>]octadéca-7(18),8,10,15-tétraén-14-ol

(5 $\alpha$ ,6 $\alpha$ )-7,8-Didehydro-4,5-epoxy-3-methoxy-17-methylmorphinan-6-ol

(5 $\alpha$ ,6 $\alpha$ )-3-Methoxy-17-methyl-7,8-didehydro-4,5-epoxymorphinan-6-ol [ACD/IUPAC Name]

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