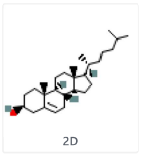
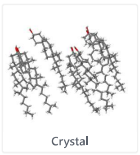
PubChem

COMPOUND SUMMARY

Cholesterol

PubChem CID	5997
Structure	 2D  3D  Crystal Find Similar Structures
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{27}H_{46}O$
Synonyms	cholesterol 57-88-5 Cholesterin Cholesteryl alcohol Cholest-5-en-3beta-ol More...
Molecular Weight	386.7
Dates	Modify 2022-10-07 Create 2004-09-16

Cholesterol is an animal sterol found in the body tissues (and blood plasma) of vertebrates. It can be found in large concentrations within the liver, spinal cord, and brain. Cholesterol is an important component of the membranes of cells, providing stability. It is the major precursor for the synthesis of vitamin D, of the various steroid hormones, including cortisol, cortisone, and aldosterone in the adrenal glands, and of the sex hormones progesterone, estrogen, and testosterone. Cholesterol also has an important role for the brain synapses as well as in the immune system. In conditions featuring elevated low density lipoproteins (LDL), cholesterol often forms plaque deposits in the walls of arteries, a condition known as atherosclerosis, which is a major contributor to coronary heart disease and other forms of cardiovascular disease.

▸ NCI Thesaurus (NCIt)

Cholesterol is a cholestanoid consisting of cholestane having a double bond at the 5,6-position as well as a 3beta-hydroxy group. It has a role as a human metabolite, a mouse metabolite, a Daphnia galeata metabolite and an algal metabolite. It is a 3beta-sterol, a cholestanoid, a C27-steroid and a 3beta-hydroxy-Delta(5)-steroid.

▸ ChEBI

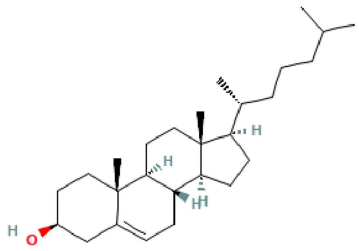
Cholesterol is a natural product found in Haplophyllum bucharicum, Bugula neritina, and other organisms with data available.

▸ LOTUS - the natural products occurrence database

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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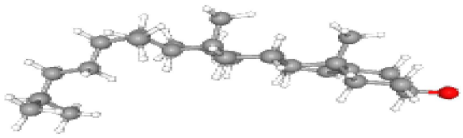
1.2 3D Conformer

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



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1.3 Crystal Structures

CCDC Number	184885
Crystal Structure Data	DOI:10.5517/cc66d1t
Crystal Structure Depiction	
Associated Article	DOI:10.1107/S0108768101018729

The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-[(2*R*)-6-methylheptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4)25(22)14-16-27(23,24)5/h9,18-19,21-25,28H,6-8,10-17H2,1-5H3/t19-,21+,22+,23-,24+,25+,26+,27-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.3 InChIKey

HVYWMOMLDIMFJA-DPAQBDIFSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric 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

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

C27H46O

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

57-88-5

CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB

22243-67-0

ChemIDplus

108598-46-5

ChemIDplus

2.3.2 Deprecated CAS

209124-38-9, 218965-24-3, 80356-14-5, 262418-13-3, 378185-03-6, 676322-57-9, 732297-95-9, 793670-51-6, 80356-33-8, 849593-11-9, 856708-55-9, 2016865-06-6, 2363129-31-9

ChemIDplus

71539-33-8

ChemIDplus

209124-38-9, 218965-24-3, 262418-13-3, 378185-03-6, 676322-57-9, 732297-95-9, 793670-51-6, 80356-14-5, 80356-33-8, 849593-11-9, 856708-55-9

EPA DSSTox

2.3.3 European Community (EC) Number

200-353-2

European Chemicals Agency (ECHA)

2.3.4 NSC Number

8798

DTP/NCI

2.3.5 UNII

97C5T2UQ7J

FDA/SPL Indexing Data

2.3.6 DSSTox Substance ID

DTXSID3022401

EPA DSSTox

2.3.7 Wikidata

Q43656

Wikidata

2.3.8 NCI Thesaurus Code

C369

NCI Thesaurus (NCIt)

2.3.9 RXCUI

2438

NLM RxNorm Terminology

2.4 Synonyms

2.4.1 MeSH Entry Terms

Cholesterol
Epicholesterol

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

cholesterol	Hydrocerin	Tegolan (VAN)	Dastar
57-88-5	Kathro	5:6-Cholesten-3beta-ol	HSDB 7106
Cholesterin	Lanol	Cholest-5-en-3-beta-ol	delta(sup 5)-
Cholesteryl alcohol	Super hartolan	Cholesterinum	Fancol CH
Cholest-5-en-3beta-ol	Provitamin D	Tegolan	3beta-Hydro
Cholestrin	Lidinite	3beta-Hydroxycholest-5-ene	Cholest-5-en
Cordulan	Cholesterol base H	Cholest-5-en-3-ol (3beta)-	NSC 8798
Dusoline	Lidinit	Cholest-5-en-3-ol	UNII-97C5T2
Dusoran	Nimco cholesterol base H	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R)-6-methylheptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	5-Cholesten-
Dythol	Wool alcohols B. P.	3-beta-Hydroxycholest-5-ene	CHEBI:16113
Cholesterine	(-)-Cholesterol	5-Cholesten-3beta-ol	AI3-03112
Cholestrol	(3beta)-cholest-5-en-3-ol	CCRIS 2834	Nimco chole

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	386.7	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3	8.7	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	5	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	386.354866087	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	386.354866087	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	20.2 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	591	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	8	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

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3.2 Experimental Properties

3.2.1 Physical Description

White or faintly yellow solid; Nearly odorless; [HSDB] Beige solid; [Sigma-Aldrich MSDS]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

Human Metabolome Database (HMDB)

3.2.2 Color/Form

White or faintly yellow pearly granules or crystals

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Almost odorless

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

3.2.4 Boiling Point

360 °C

PhysProp

DrugBank

360.0 °C

EPA DSSTox

360 °C (decomposes)

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

3.2.5 Melting Point

148.5 °C

PhysProp

DrugBank

145.0 °C

EPA DSSTox

148.5 °C

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

MP: 145.5 °C (the melt becomes clear at 180 °C); optical rotation (25 °C/D) = -13.7 deg (c = 0.9 in chloroform) /Benzoate/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 381

Hazardous Substances Data Bank (HSDB)

148 °C

Human Metabolome Database (HMDB)

3.2.6 Solubility

0.095 mg/L (at 30 °C)

YALKOWSKY,SH & DANNENFELSER,RM (1992)

DrugBank

2.46e-07 M

YALKOWSKY,SH & DANNENFELSER,RM (1992)

EPA DSSTox

Moderately soluble in hot alcohol; soluble in benzene, oils, fats and aq solns of bile salts

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

In water, 0.095 mg/l @ 30 °C.

Yalkowsky SH, Dannenfelser RM; The AQUASOL dATAbASE of Aqueous Solubility. Ver 5. Tucson, AZ: Univ AZ, College of Pharmacy (1992)

Hazardous Substances Data Bank (HSDB)

9.5e-05 mg/mL

Human Metabolome Database (HMDB)

3.2.7 Density

1.067 @ 20 °C/4 °C

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

Pearly leaflets or plates from dilute alcohol; becomes anhydrous at 70-80 °C; density 1.03; practically insoluble in water (about 0.2 mg/100 ml H2O); slightly soluble in alcohol (1.29% w/w at 20 °C); more soluble in hot alcohol (100 g of saturated 96% alcoholic solution contains 28 g at 80 °C); one gram dissolves in 2.8 ml ether, in 4.5 ml chloroform, in 1.5 ml pyridine. Also soluble in benzene petroleum, oils, fats. Soluble in aqueous solution of bile salts; optical rotation (20 °C/D) = -31.5 deg (c = 2 in ether); optical rotation (20 °C/D) = -39.5 deg (c= 2 in chloroform). /Monohydrate/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 381

Hazardous Substances Data Bank (HSDB)

3.2.8 Vapor Pressure

VP: 0.171 mm Hg at 149 °C

Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, DC: Taylor and Francis (2001)

Hazardous Substances Data Bank (HSDB)

3.2.9 Optical Rotation

Specific rotation: -34 to 38 deg @ 25 °C

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 265

Hazardous Substances Data Bank (HSDB)

3.2.10 Decomposition

When heated to decomposition it emit acrid smoke and irritating fumes.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 848

Hazardous Substances Data Bank (HSDB)

3.2.11 Collision Cross Section

204.6 Å² [M+H]⁺ [CCS Type: TW, Method: calibrated with polyalanine and drug standards]

https://pubs.acs.org/doi/abs/10.1021/acs.analchem.7b01709

▸ CCSbase

3.2.12 Other Experimental Properties

Crystal from acetone; MP 84 °C; optical rotation (20 °C/D) = -45.8 deg (c = 1.2 in chloroform). /Methyl ether/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 381

▸ Hazardous Substances Data Bank (HSDB)

Needles from acetone; MP 115-116 °C; optical rotation (20 dec C/D) = -47.4 deg (c = 2 in chloroform). /Acetate/

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 381

▸ Hazardous Substances Data Bank (HSDB)

3.2.13 Chemical Classes

Biological Agents -> Cholesterol and Derivatives

▸ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.3 SpringerMaterials Properties

Boiling point	Heat capacity	Surface tension
Chemical diffusion	Heat of sublimation	Thermal conductivity
Compressibility	High frequency properties	Transition enthalpy
Corrosion	Magnetic susceptibility	Transparency
Crystal structure	Melting temperature	Unit cell
Crystallographic data	Order parameter	Unit cell parameter
Density	Phase transition	Vapor pressure
Diamagnetic susceptibility	Point group	Viscosity
Dielectric permittivity	Polarizability	
Dielectric susceptibility	Refractive index	
Diffusive flux	Second-order nonlinear coefficient	
Formula unit	Sound velocity	
Fusion temperature	Space group	

▸ SpringerMaterials