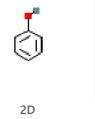
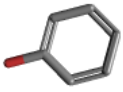
PubChem

RESUMEN COMPUESTO

Fenol

PubChem CID	996
Estructura	 2D  3D  Crystal Encuentra estructuras similares
Seguridad química	 Corrosive Acute Toxic Health Hazard Hoja de datos del resumen de seguridad química de laboratorio (LCSS)
Fórmula molecular	C_6H_5OH o C_6H_6O
Sinónimos	fenol 108-95-2 ácido carbólico Hidroxibenceno Ácido fenico Más...
Peso molecular	94,11 g / mol
Fecha s	Modificar 2021-01-31 Crear 2004-09-16

El fenol es un producto químico fabricado y una sustancia natural. Es un sólido de incoloro a blanco cuando está puro. El producto comercial es un líquido. El fenol tiene un olor distintivo que es repugnantemente dulce y alquitranado. Puede saborear y oler el fenol a niveles más bajos que los asociados con efectos nocivos. El fenol se evapora más lentamente que el agua y una cantidad moderada puede formar una solución con agua . El fenol puede incendiarse. El fenol se utiliza principalmente en la producción de resinas fenólicas y en la fabricación de nailon y otras fibras sintéticas. También se utiliza en anticoagulantes (productos químicos que matan bacterias y hongos en los lodos), como desinfectante y antiséptico, y en preparaciones medicinales como enjuagues bucales y pastillas para el dolor de garganta.

▸ Portal de sustancias tóxicas de CDC-ATSDR

Phenol, liquid appears as a colorless liquid when pure, otherwise pink or red. Combustible. Flash point 175°F. Must be heated before ignition may occur easily. Vapors are heavier than air. Corrosive to skin but because of anesthetic qualities will numb rather than burn. Upon contact skin may turn white. May be lethal by skin absorption. Does not react with water. Stable in normal transportation. Reactive with various chemicals and may be corrosive to lead, aluminum and its alloys, certain plastics, and rubber. Freezing point about 105°F. Density 8.9 lb / gal. Used to make plastics, adhesives and other chemicals.

▸ CAMEO Chemicals

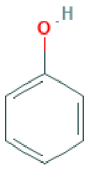
Phenol is an organic hydroxy compound that consists of benzene bearing a single hydroxy substituent. The parent of the class of phenols. It has a role as a disinfectant, an antiseptic drug, a human xenobiotic metabolite and a mouse metabolite. It is a conjugate acid of a phenolate.

▸ ChEBI

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Conformer

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1.3 Crystal Structures

Showing 1 of 2 View More

CCDC Number	201623
Crystal Structure Data	DOI:10.5517/cc6rszp
Crystal Structure Depiction	
Associated Article	DOI:10.1107/S0108768102018797

The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

phenol

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

PubChem

2.1.2 InChI

InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.3 InChI Key

ISWSIDIOOBJBQZ-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.4 Canonical SMILES

C1=CC=C(C=C1)O

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

2.2 Molecular Formula

C6H5OH

CAMEO Chemicals; Wikipedia

C6H6O

CAMEO Chemicals; PubChem

C6H6O

C6H5OH

ILO International Chemical Safety Cards (ICSC)

2.3 Other Identifiers

2.3.1 CAS

108-95-2

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

61788-41-8

ChemIDplus; EPA Chemicals under the TSCA; European Chemicals Agency (ECHA)

63496-48-0

ChemIDplus

73607-76-8

ChemIDplus

2.3.2 Related CAS

139-02-6 (hydrochloride salt)

ChemIDplus

2.3.3 Deprecated CAS

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

ChemIDplus

2.3.4 European Community (EC) Number

203-632-7

European Chemicals Agency (ECHA)

262-972-4

European Chemicals Agency (ECHA)

2.3.5 ICSC Number

0070

ILO International Chemical Safety Cards (ICSC)

2.3.6 NSC Number

36808

DTP/NCI

2.3.7 RTECS Number

SJ3325000

The National Institute for Occupational Safety and Health (NIOSH)

2.3.8 UN Number

2821

CAMEO Chemicals; DOT Emergency Response Guidebook; The National Institute for Occupational Safety and Health (NIOSH)

2312

CAMEO Chemicals; DOT Emergency Response Guidebook; The National Institute for Occupational Safety and Health (NIOSH)

1671

CAMEO Chemicals; DOT Emergency Response Guidebook; ILO International Chemical Safety Cards (ICSC); NJDOH RTK Hazardous Substance List; The National Institute for Occupational Safety and Health (NIOSH)

2.3.9 UNII

339NCG44TV

FDA/SPL Indexing Data

2.3.10 FEMA Number

3223

Flavor and Extract Manufacturers Association (FEMA)

2.3.11 DSSTox Substance ID

DTXSID5021124

EPA DSSTox

2.3.12 Wikipedia

Phenol

Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

Carbol
Carbolic Acid
Hydroxybenzene
Phenol

Phenol, Sodium Salt
Phenolate Sodium
Phenolate, Sodium
Sodium Phenolate

MeSH

2.4.2 Depositor-Supplied Synonyms

phenol	PhOH	Fenosmoline	Phenic	UN 1671 (solid)	UNII-339NCG44TV	339NCG44TV
108-95-2	Monohydroxybenzene	Phenosmolin	Carbolsaure [German]	Phenol [JAN]	UN1671	DTXSID5021124
carbolic acid	Paoscle	Fenol	Campho-Phenique Liquid	Caswell No. 649	UN2312	CHEBI:15882
Hydroxybenzene	Phenole	Liquid phenol	NCI-C50124	NSC 36808	UN2821	Phenol (or solutions with 5%
Phenic acid	Izal	Carbolic oil	Phenol, molten	Campho-Phenique Cold Sore Gel	CCRIS 504	NSC-36808
Oxybenzene	Phenol alcohol	Phenol, pure	Baker's P & S liquid & Ointment	Phenic alcohol	FEMA No. 3223	Hydroxybenzene solution
Phenylic acid	Phenyl alcohol	Phenol homopolymer	Fenol [Dutch, Polish]	Liquefied phenol	HSDB 113	Phenol, solid [UN1671] [Poisc
Benzenol	Phenol, liquefied	Fenolo [Italian]	Baker's P and S Liquid and Ointment	Synthetic phenol	AI3-01814	Phenol, molten [UN2312] [Pc
Monophenol	Acide carbolique	Phenole [German]	Monohydroxy benzene	Phenol, liquid	EINECS 203-632-7	NCGC00091454-04
Phenyl hydrate	Fenolo	Benzene, hydroxy-	Un 2812 (solution)	Phenol, solid	MFCD00002143	Phenol solutions [UN2821] [F
Phenylic alcohol	Carbolsaure	Rcra waste number U188	UN 2312 (molten)	RCRA waste no. U188	EPA Pesticide Chemical Code 064001	DSSTox_CID_1124
Phenyl hydroxide	Fenosmolin	Campho-Phenique Gel	Acide carbolique [French]	Baker's p and s	CHEMBL14060	Phenol, >=99.0%

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	94.11 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3	1.5	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	94.041865 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	94.041865 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	20.2 Å²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	7	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	46.1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	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 2019.01.04)

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3.2 Experimental Properties

3.2.1 Physical Description

Phenol solution, [aqueous] is a white crystalline mass dissolved in an aqueous solution. Solution may be colorless to slightly pink in color with a distinctive phenol odor; sharp burning taste. Aqueous solution will be acidic and act as such. Toxic by ingestion, inhalation and skin absorption; strong irritant to tissues.

CAMEO Chemicals

Phenol, liquid appears as a colorless liquid when pure, otherwise pink or red. Combustible. Flash point 175°F. Must be heated before ignition may occur easily. Vapors are heavier than air. Corrosive to skin but because of anesthetic qualities will numb rather than burn. Upon contact skin may turn white. May be lethal by skin absorption. Does not react with water. Stable in normal transportation. Reactive with various chemicals and may be corrosive to lead, aluminum and its alloys, certain plastics, and rubber. Freezing point about 105°F. Density 8.9 lb / gal. Used to make plastics, adhesives and other chemicals.

CAMEO Chemicals

Phenol, molten is the white crystalline solid shipped at an elevated temperature to form a semi-solid. It is very hot and may cause burns from contact and also may cause the ignition of combustible materials. It is toxic by ingestion, and inhalation of its fumes, and skin absorption. It may also be very irritating to skin and eyes. It is used to make other chemicals.

CAMEO Chemicals

Phenol, solid appears as a solid melting at 110°F. Colorless if pure, otherwise pink or red. Flash point 175°F. Density 9.9 lb / gal. Vapors are heavier than air Corrosive to the skin (turning skin white) but because of its anesthetic quality numbs rather than burn. Lethal amounts can be absorbed through the skin. Used to make plastics and adhesives.

CAMEO Chemicals

DryPowder; Liquid; PelletsLargeCrystals, Liquid; PelletsLargeCrystals, OtherSolid

EPA Chemicals under the TSCA

Solid

Human Metabolome Database (HMDB)

COLOURLESS-TO-YELLOW OR LIGHT PINK CRYSTALS WITH CHARACTERISTIC ODOUR.

ILO International Chemical Safety Cards (ICSC)

White crystalline mass, sharp, medicinal, sweet, tarry odour

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Colorless to light-pink, crystalline solid with a sweet, acrid odor.

Occupational Safety and Health Administration (OSHA)

Colorless to light-pink, crystalline solid with a sweet, acrid odor. [Note: Phenol liquefies by mixing with about 8% water.]

The National Institute for Occupational Safety and Health (NIOSH)