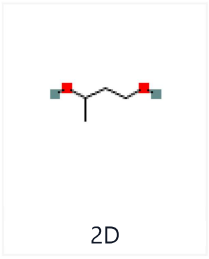
COMPOUND SUMMARY

1,3-Butanediol

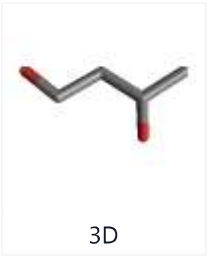
PubChem CID

7896

Structure



2D



3D

Chemical Safety

Flammable

Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula

$C_4H_{10}O_2$

$CH_3CHOHCH_2CH_2OH$

Synonyms

1,3-BUTANEDIOL

Butane-1,3-diol

107-88-0

1,3-Butylene glycol

Butylene glycol

View More...

Molecular Weight

90.12 g/mol

Computed by PubChem 2.1 (PubChem release 2021.05.07)

Dates

Create:	Modify:
2005-03-26	2023-07-29

Description

Butane-1,3-diol is a butanediol compound having two hydroxy groups in the 1- and 3-positions. It is a butanediol and a glycol.

▸ ChEBI

1,3-Butanediol is found in pepper (c. annuum). 1,3-Butanediol is a solvent for flavouring agents 1,3-Butanediol is an organic chemical, an alcohol. It is commonly used as a solvent for food flavouring agents and is a co-monomer used in certain polyurethane and polyester resins. It is one of four stable isomers of butanediol. In biology, 1,3-butanediol is used as a hypoglycaemic agent. 1,3-Butanediol belongs to the family of Secondary Alcohols. These are compounds containing a secondary alcohol functional group, with the general structure HOC(R)(R') (R,R'=alkyl, aryl).

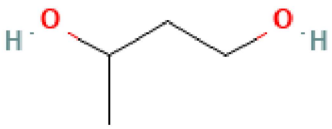
▸ Toxin and Toxin Target Database (T3DB)

Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction



PubChem

1.2 3D Conformer

UPDATING...

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

butane-1,3-diol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

2.1.2 InChI

InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.3 InChIKey

PUPZLCDOIYMWBV-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

2.1.4 Canonical SMILES

CC(CCO)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

$C_4H_{10}O_2$

$CH_3CHOHCH_2CH_2OH$

ILO-WHO International Chemical Safety Cards (ICSCs)

$C_4H_{10}O_2$

Computed by PubChem 2.1 (PubChem release 2021.05.07)

- Wikipedia; PubChem

2.3 Other Identifiers

2.3.1 CAS

107-88-0

- CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; ...

2.3.2 Related CAS

55251-78-0

Compound: 1,3-Butanediol polymer

- CAS Common Chemistry

2.3.3 Deprecated CAS

18826-95-4, 817176-75-3

- ChemIDplus

817176-75-3

- EPA DSSTox

2.3.4 European Community (EC) Number

203-529-7

- European Chemicals Agency (ECHA)

2.3.5 ICSC Number

1182

- ILO-WHO International Chemical Safety Cards (ICSCs)

2.3.6 NSC Number

402145

- DTP/NCI