

Product Safety Summary for Pentanediol

SUBSTANCE NAME

Pentanediol
1,5-Pentandiol
1,5-Pentanediol
1,5-Pentanediol (8CI, 9CI)
Pentane-1,5-diol
1,5- Dihydroxypentane
Pentamethyleneglycol
1,5-Pentamethylene glycol
Pentyleneglycol
omega.-Pentanediol
alpha.,omega.-Pentanediol

GENERAL STATEMENT

Pentanediol is a colorless, odorless liquid. It is neither hazardous for human health nor for the environment. Pentanediol has a wide range of applications. It has two functional groups which are useful in the production of various polymers and plastic products. But it also finds application in other chemical processes as well as it is contained in different consumer products.

CHEMICAL IDENTITY

EC Name: pentane-1,5-diol
EC-No. : 203-854-4
CAS-No. : 111-29-5
Molecular formula: C₅H₁₂O₂
Structural formula:



USES AND APPLICATIONS

Pentanediol is obtained after treatment of the mixture of products resulting from the oxidation of cyclohexane with air. Pentanediol is used to produce materials made of polyester or polyurethane, for the manufacturing of monomers, for the manufacture of polyester polyols, polycarbonatedioles and acrylic monomers, for the production of delta valerolactone and for molecules that act as reactive diluents, for the production of halogenated substances and for the production of adhesives, putties and sealing compounds, cleaners and auxiliary agents. Pentanediol is also used in the processes to produce hydrogen, hydrogen peroxide, sodium perborate and peroxyacetic acid and as an intermediate for pharmaceutical products. It is used as an ingredient for the production of polymeric thickeners, plasticizers for polyvinyl chloride, sizing agents, surfactants, for starches and chemically modified starch for application in the paper, textile and food industry, for personal hygiene products like shampoo, creams, and for paints.

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PHYSICAL CHEMICAL PROPERTIES

Pentanediol is a colorless and odorless liquid at room temperature.

Melting point/range:	ca. -16 °C
Boiling point/boiling range:	238 °C at 1013.25 hPa
Decomposition temperature:	Not determined
Flashpoint:	142 °C (closed cup)
Flammability (solid, gaseous):	Not flammable upon ignition
Autoignition temperature:	330 °C
Explosion limits:	
Lower:	1.3 %
Upper:	13.2 %
Explosive properties:	Non explosive.
Molecular weight:	104.1476 g/mol
log Pow:	-0.49 at 25 °C
Vapor pressure:	0.0052 hPa at 25 °C
Relative density:	0.985 g/cm ³ at 25.2 °C
Solubility in/Miscibility with water:	Miscible in any ratio at 20 °C
Oxidizing properties:	No oxidizing properties

HEALTH EFFECTS

Pentanediol has no marked health hazard properties. Its acute toxicity is very low via all routes of exposure tested (oral, skin and inhalation). It has no irritation or sensitization effects. Limited repeated dose and long term health or reproductive effects has been generated with Pentanediol itself. More extensive data is available for the analogous substance Hexanediol. Based on the total amount of information available Pentanediol is not expected to cause repeated dose or long term health effects. The physical properties of Pentanediol give no rise to concern. Its flammability is low. Therefore, Pentanediol has a very low overall human health hazard potential.

EFFECT ASSESSMENT	RESULT
Acute Toxicity (oral/dermal/inhalation)	Pentanediol is of low acute toxicity via all routes of exposure.
Irritation/Corrosivity (skin/eye/respiratory tract)	Pentanediol is not irritating to the skin or to the eyes. Corrosivity was not tested on the basis of the absence of irritation properties.
Sensitization (skin/respiratory tract)	Based on the available data, Pentanediol is not considered to have skin or respiratory sensitization properties.
Repeated Dose Exposure	Oral repeated dose test results with an analogous substance (Hexanediol) suggest that no marked toxicity should be expected. Dermal and inhalation repeated dose exposure testing is considered unnecessary based on expected exposure routes and the oral repeated dose test result.
Mutagenicity	All available in vitro test data on Pentanediol and the analogous Hexanediol indicates that bioaccumulation is not expected.
Carcinogenicity	No carcinogenicity data has been generated due to the negative mutagenicity results.
Reproductive Toxicity	Screening test information with the analogous Hexanediol suggests Pentanediol should have no adverse reprotoxicity effects either.

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ENVIRONMENTAL EFFECTS

The results of all three acute aquatic studies on fish, algae, plants and invertebrates indicate a low environmental acute hazard potential for Pentanediol. Pentanediol is readily biodegradable and it has a very low bioaccumulation potential. Considering all available data on biotic and abiotic degradation, bioaccumulation and toxicity, it can be stated that the substance is neither persistent nor toxic to the environment and that it will not bio-accumulate. Overall Pentanediol has a very low environmental hazard potential.

EFFECT ASSESSMENT	RESULT
Aquatic Toxicity	Fish, daphnia, algae and plants studies indicate that the aquatic toxicity of Pentanediol is low.

FATE AND BEHAVIOR	RESULT
Biodegradation	Pentanediol is readily biodegradable, based on test results with Pentanediol itself and analogous substances (Hexanediol and Butanediol).
Bioaccumulation potential	Pentanediol will preferentially distribute to water. Based on the value of the partition coefficient it is concluded that bioaccumulation is not expected.
PBT/vPvB conclusion	Based on its low toxicity, bioaccumulation potential and ready biodegradability, Pentanediol does not meet the criteria for PBT or vPvB.

EXPOSURE

Human Health

Pentanediol is used in many different applications. In industrial sites it is used for the production of hydrogen, hydrogen peroxide, sodium perborate and peroxyacetic acid. But its main industrial use is as monomer or reactant, therefore, Pentanediol will no longer be present as such in downstream products, practically eliminating the exposure potential for professional users and consumers.

On the other hand, Pentanediol is contained in formulated products of common use, such as adhesives, putties, sealing compounds, cleaners, paints and inks, synthetic resins and personal hygiene products (shampoo, creams, etc.). In all previous cases, Pentanediol occurs in diluted form, so professionals and consumers level of exposure will be very low.

Environment

Pentanediol is liquid at room temperature and it has relatively low volatility. The probability of release in pure form to any of the environmental compartments is low under normal industrial use conditions. There may be some release to waste water streams as a result of normal use or industrial cleaning operations, but, as Pentanediol is readily biodegradable, this should not cause further environmental exposure.

RISK MANAGEMENT RECOMMENDATIONS

Pentanediol poses very low human health and environmental risks. However, it is a good practice to train personnel handling the substance and to protect workers who may be exposed to Pentanediol by taking the usual precautionary measures to protect against chemical exposure. Therefore, protective clothing, gloves and safety glasses with side shields should be worn when handling this substance. Good ventilation is required in areas where Pentanediol is handled. Respiratory protection is not required unless pentanediol is

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released in the form of gas or in the form of aerosols. Pentanediol is not flammable, however, it is a good practice to prevent the build-up of electrostatic charge when storing it.
For environmental protection in case of accidental release: do not allow product to reach sewage system or any water course. Retain and dispose of contaminated wash water.

STATE AGENCY REVIEW

This substance has been registered under REACH (EC) No. 1907/2006.
Pentanediol is included in the OECD list of High Production Volume (HPV) chemicals, but a SIDS is not yet available.
Pentanediol is listed in the following Chemical Inventories: AICS, NZIoC, KECl, PICCS, IECSC, EINECS, Canada DSL, TSCA, ENCS.

REGULATORY INFORMATION/CLASSIFICATION AND LABELING

Classification of the substance according to REGULATION (EC) No 1272/2008:

Not classified.

Labeling according to REGULATION (EC) No 1272/2008:

Pictogram: none

Signal word: none

Hazard statements: none

CONTACT INFORMATION WITHIN COMPANY

For further information on this substance or product safety summaries in general, please contact:

Company:	UBE Chemical Europe, S.A
Department:	Corporate Social Responsibility
Address:	Poligono Industrial El Serrallo, s/n
Town/Country:	Grao de Castellon (Castellon), Spain
Postal code:	12100
E-mail:	sds.ube.eu@ube.es

Additional information can be found at:

<http://www.ube.es>

<http://www.icca-chem.org/en/Home/ICCA-initiatives/global-product-strategy/>

GLOSSARY

Acute toxicity	Harmful effect resulting from a single or short term exposure to a substance.
AICS	Australian Inventory of Chemical Substances.
Biodegradation	Decomposition or breakdown of a substance under natural conditions (actions of micro-organisms etc).
Bioaccumulation	Progressive accumulation in living organisms of a

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Canadian DSL	chemical substance present in the environment.
Carcinogenicity	Domestic Substances List of Canada.
CAS	Substance effects causing cancer.
Chronic toxicity	Chemical Abstracts Service (division of the American Chemical Society).
EINECS	Harmful effect after repeated exposures or long term exposure to a substance.
ENCS	European Inventory of Existing Commercial Chemical Substances
Flash point	Existing Notified Chemical Substances (Japan).
Genotoxicity	The lowest temperature at which vapor of the substance may form an ignitable mixture with air.
GHS	Substance effect that causes damage to genes, including mutagenicity and clastogenicity.
HPV	Globally Harmonized System of Classification and Labeling of Chemicals
Hydrolyze	High Production Volume Chemicals.
IECSC	Undergo hydrolysis; decompose by reacting with water.
Intermediate	Inventory of Existing Chemical Substances Produced or Imported in China.
KECI	Substance that is manufactured for and consumed in or used for chemical processing in order to be transformed into another substance.
Monomer	Korean Existing Chemical Inventory.
Mutagenicity	Means a substance which is capable of forming covalent bonds with a sequence of additional like or unlike molecules under the conditions of the relevant polymer-forming reaction used for the particular process.
NZIoC	Substance effect that cause mutation on genes.
PBT	New Zealand Inventory of Chemicals
Persistence	Persistent, bioaccumulative, toxic chemical.
PICCS	Refers to the length of time a compound stays in the environment, once introduced.
Risk Management Measures	Philippine Inventory of Chemicals and Chemical Substances.
REACH (EC) No. 1907/2006	Engineering controls, conditions and protective equipment needed to be implemented to ensure that the risks to human health and the environment are adequately controlled.
REGULATION (EC) No 1272/2008	European Commission Regulation concerning the Registration, Evaluation, Authorization and Restriction of Chemicals.
Reprotoxicity	European Commission Regulation on Classification, Labeling and Packaging of Substances and Mixtures.
Sensitizing	Including teratogenicity, embryotoxicity and harmful effects on fertility.
Sediment	Allergenic.
	Topsoil, sand and minerals washed from land into water forming in the end a layer at the bottom of rivers and sea.

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TSCA

Toxic Substance Control Act (USA).

Vapor pressure

A measure of a substance's property to evaporate.

vPvB

Very persistent, very bio-accumulative.

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REVISION

Version 1.0

DISCLAIMER

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