

Chemical Safety Data Sheet MSDS / SDS

1-PHENYLETHANOL-1,2-13C2

Revision Date:2026-05-31 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : 1-PHENYLETHANOL-1,2-13C2
CBnumber : CB5777154
CAS : 285138-87-6
Synonyms : 1-Phenylethanol-1,2-13C?;sec-phenethyl- α,β -13c2alcohol

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

Precautionary statements

P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.

Hazard statements

H302 Harmful if swallowed
H315 Causes skin irritation
H318 Causes serious eye damage

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-PHENYLETHANOL-1,2-13C2
Synonyms	: 1-Phenylethanol-1,2-13C?;sec-phenethyl- α,β -13c2alcohol
CAS	: 285138-87-6
MF	: C8H10O
MW	: 124.18

SECTION 4: First aid measures

General advice

Show this safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Combustible. Vapours are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating. Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

Carbon oxides

Specific extinguishing methods

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

In the event of fire, wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Storage

Further information on storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class

6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

Recommended storage temperature

Recommended storage temperature see product label.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection

protective clothing

Hand protection

Remarks

required

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

No data available

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

-27 °C

Boiling point/boiling range

219 - 221 °C (1,000 hPa)

Flash point

85 °C

Method: closed cup

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

1.040 g/mL at 25 °C

Density

1.03 g/cm³ (25 °C)

Water solubility

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

none

Molecular weight

124.14 g/mol

Particle characteristics Particle size

No data available

SECTION 10: Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with: Strong acids Strong oxidizing agents

Conditions to avoid

Strong heating.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

LD50 Dermal - Rabbit - female - > 2,000 mg/kg (OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: (±)-α- methylbenzyl alcohol

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: (±)-α- methylbenzyl alcohol

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes. - 24 h (OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: (±)-α- methylbenzyl alcohol

Respiratory or skin sensitization

Draize Test - Guinea pig

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: (±)-α-methylbenzyl alcohol

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: (±)-α- methylbenzyl alcohol
Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: (±)-α- methylbenzyl alcohol

Test Type: In vivo micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: (\pm)- α -methylbenzyl alcohol

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Repeated dose toxicity - Mouse - male and female - Oral - 16 Days - No observed adverse effect level - 500 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: (\pm)- α -methylbenzyl alcohol

After absorption of large quantities:

Possible symptoms:

Nausea

Vomiting

Dizziness

Damage to:

Cardiac

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

Ecotoxicity

Components:

1-Phenylethanol-1,2-13C2:

Toxicity to fish

LC50 (Danio rerio (zebra fish)): > 100 mg/l End point: mortality Exposure time: 96 h Test Type: static test Method: OECD Test Guideline 203

Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: (\pm)- α -methylbenzyl alcohol

Toxicity to algae/aquatic plants

ErC50 (Chlorella vulgaris (Fresh water algae)): > 200 mg/l Exposure time: 72 h Test Type: static test Method: OECD Test Guideline 201

Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: (\pm)- α -methylbenzyl alcohol

Persistence and degradability

Components:

1-Phenylethanol-1,2-13C2:

Biodegradability

aerobic Inoculum: activated sludge, adapted Concentration: 100 mg/l Result: Readily biodegradable. Biodegradation: 100 % Exposure time: 28 d Remarks: (ECHA) The value is given in analogy to the following substances: The value is given in analogy to the following substances: (±)-α-methylbenzyl alcohol

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

Components:

1-Phenylethanol-1,2-13C2:

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 2937

Proper shipping name : alpha-Methylbenzyl alcohol, liquid

Class : 6.1

Packing group : III

Labels : Division 6.1 - Toxic substances

Packing instruction (cargo aircraft) : 663

Packing instruction (passenger aircraft) : 655

IMDG-Code

UN number : UN 2937

Proper shipping name : alpha-METHYLBENZYL ALCOHOL, LIQUID

Class : 6.1

Packing group : III

Labels : 6.1

EmS Code : F-A, S-A

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

JT/T 617

UN number : UN 2937

Proper shipping name : ALPHA-METHYLBENZYL ALCOHOL, LIQUID

Class : 6.1

Packing group : III

Labels : 6.1

Environmentally hazardous : no

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

Listed

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Not listed

Hazardous Chemicals for Priority Management

Not listed under SAWS

Catalogue of Specially Controlled Hazardous

Not listed Chemicals

List of Explosive Precursors

Not listed

Regulations on Labour Protection in Workplaces where Toxic Substances are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222243399

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

Regulations on the Administration of Controlled Chemicals

List of Controlled Chemicals

Not listed

Regulations of Ozone Depleting Substances Management

List of Controlled Ozone Depleting Substances

Not listed

List of Controlled Ozone Depleting Substances Import and Export

Not listed

Environmental Protection Law

List of Priority Controlled Chemicals

Not listed

List of Key Controlled New Pollutants

Not listed

SECTION 16: Other information

Full text of other abbreviations

AIIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCs - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonised System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC₅₀ - Half maximal inhibitory concentration

ICAO - International Civil Aviation Organization

IECSC - Inventory of Existing Chemical Substances in China

IMDG - International Maritime Dangerous Goods

IMO - International Maritime Organisation

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardisation

KECI - Korea Existing Chemicals Inventory

LC₅₀ - Lethal Concentration to 50 % of a test population

LD₅₀ - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pollution from Ships

MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods

n.o.s. - Not Otherwise Specified

NCh - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NOM - Official Mexican Norm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chemicals

OECD - Organisation for Economic Co-operation and Development

OPPTS - Office of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Substances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - Taiwan Chemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI - Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (United States)

UN - United Nations

UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.