

Chemical Safety Data Sheet MSDS / SDS

1-Eth-1-ynyl-4-(pentyloxy)benzene

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-Eth-1-ynyl-4-(pentyloxy)benzene
CBnumber : CB2491721
CAS : 79887-16-4
Synonyms : 4-N-PENTYLPHENYLACETYLENE, 1-Eth-1-ynyl-4-(pentyloxy)benzene

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

Warning

Precautionary statements

P233 Keep container tightly closed.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P304 IF INHALED:
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.

P312 Call a POISON CENTER or doctor/physician if you feel unwell.

P321 Specific treatment (see ... on this label).

P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P340 Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P362 Take off contaminated clothing and wash before reuse.

P403 Store in a well-ventilated place.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

P501 Dispose of contents/container to....

Hazard statements

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-Eth-1-ynyl-4-(pentyloxy)benzene
Synonyms	: 4-N-PENTYLPHENYLACETYLENE, 1-Eth-1-ynyl-4-(pentyloxy)benzene
CAS	: 79887-16-4
MF	: C13H16O
MW	: 188.27

SECTION 4: First aid measures

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.

Inhalation

Remove to fresh air. Get medical attention immediately if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Most important symptoms and effects

None reasonably foreseeable.

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

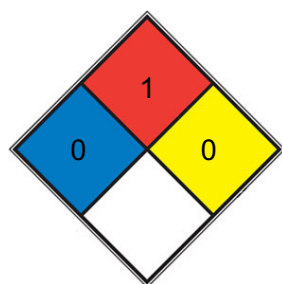
Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA 704



■ HEALTH	0	Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials
■ FIRE	1	Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. mineral oil , ammonia)
■ REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
□ SPEC.		
□ HAZ.		

SECTION 6: Accidental release measures

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal.
Refer to protective measures listed in Sections 8 and 13.

SECTION 7: Handling and storage

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation.

Storage

Keep container tightly closed in a dry and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8: Exposure controls/personal protection

Control Parameters

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 96

Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

Engineering Measures

None under normal use conditions. .

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g.

sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection

Long sleeved clothing

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Colorless

Physical State

Liquid

Odor

No information available

Odor Threshold

No data available

pH

No information available

Melting Point/Range

No data available

Softening Point

No data available

Boiling Point/Range

113 - 115 °C / 235.4 - 239 °F

Flash Point

> 110 °C / > 230 °F Method - No information available

Evaporation Rate

No data available

Flammability (solid,gas)

Not applicable Liquid

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

No data available (Air = 1.0)

Specific Gravity / Density

0.96±0.1 g/cm³(Predicted)

Bulk Density

Not applicable Liquid

Water Solubility

Immiscible

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

Autoignition Temperature

No data available

Decomposition Temperature

No data available

Viscosity

No data available

Explosive Properties

No information available

Oxidizing Properties

No information available

Molecular Formula

C13 H16 O

Molecular Weight

188.27

SECTION 10: Stability and reactivity

Stability

Stable under normal conditions.

Hazardous Reactions

None under normal processing.

Hazardous Polymerization

No information available.

Conditions to Avoid

None known.

Materials to avoid

No information available.

Hazardous Decomposition Products

None under normal use conditions.

SECTION 11: Toxicological information

Product Information

(a) acute toxicity;

(b) skin corrosion/irritation;

No data available

(c) serious eye damage/irritation;

No data available

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

No data available

(h) STOT-single exposure;

No data available

(i) STOT-repeated exposure;

No data available

Target Organs

No information available.

(j) aspiration hazard;

No data available

Symptoms / effects, both acute and delayed

No information available

SECTION 12: Ecological information

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability

Persistence

Immiscible with water, Persistence is unlikely, based on information available.

Bioaccumulative Potential

May have some potential to bioaccumulate

Mobility in soil

Spillage unlikely to penetrate soil The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility Will likely be mobile in the environment due to its volatility

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

This product does not contain any known or suspected substance

Ozone Depletion Potential

This product does not contain any known or suspected substance

SECTION 13: Disposal considerations

Waste from Residues/Unused Products

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Contaminated Packaging

Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14: Transport information

Road and Rail Transport

Not Regulated

IMDG/IMO

Not regulated

IATA

Not regulated

Special Precautions for User

No special precautions required

SECTION 15: Regulatory information

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCS	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
1-Eth-1-ynyl-4-(pentyloxy)benzene	-	-	X	-	-	-	-	-	-	-	-	-

National Regulations

SECTION 16: Other information

Prepared By

Health, Safety and Environmental Department

Revision Date

24-Sep-2025

Revision Summary

Not applicable.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Legend

CAS

Chemical Abstracts Service

TSCA

United States Toxic Substances Control Act Section 8(b)

Inventory

EINECS/ELINCS

European Inventory of Existing Commercial Chemical

Substances/EU List of Notified Chemical Substances

DSL/NDSL

Canadian Domestic Substances List/Non-Domestic

Substances List

PICCS

Philippines Inventory of Chemicals and Chemical Substances

ENCS

Japanese Existing and New Chemical Substances

IECSC

Chinese Inventory of Existing Chemical Substances

AICS

Australian Inventory of Chemical Substances

KECL

Korean Existing and Evaluated Chemical Substances

NZIoC

New Zealand Inventory of Chemicals

WEL

Workplace Exposure Limit

TWA

Time Weighted Average

ACGIH

American Conference of Governmental Industrial Hygienists

IARC

International Agency for Research on Cancer

DNEL

Derived No Effect Level

PNEC

Predicted No Effect Concentration

RPE

Respiratory Protective Equipment

LD50

Lethal Dose 50%

LC50

Lethal Concentration 50%

EC50

Effective Concentration 50%

NOEC

No Observed Effect Concentration

POW

Partition coefficient Octanol:Water

PBT

Persistent, Bioaccumulative, Toxic

vPvB

very Persistent, very Bioaccumulative

ICAO/IATA

International Civil Aviation Organization/International Air
Transport Association

IMO/IMDG

International Maritime Organization/International Maritime
Dangerous Goods Code

ADR

European Agreement Concerning the International Carriage of

Dangerous Goods by Road

MARPOL

International Convention for the Prevention of Pollution from

Ships

OECD

Organisation for Economic Co-operation and Development

ATE

Acute Toxicity Estimate

BCF

Bioconcentration factor

VOC

(Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

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.