

Chemical Safety Data Sheet MSDS / SDS

1,5-HEXADIYNE

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

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

Product name : 1,5-HEXADIYNE
CBnumber : CB8778536
CAS : 628-16-0
EINECS Number : 211-029-5
Synonyms : 1,5-hexadiyne,hexa-1,5-diyne

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

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.
P405 Store locked up.

Hazard statements

H225 Highly Flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H319 Causes serious eye irritation

H336 May cause drowsiness or dizziness

H411 Toxic to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

Product name : 1,5-HEXADIYNE
Synonyms : 1,5-hexadiyne,hexa-1,5-diyne
CAS : 628-16-0
EC number : 211-029-5
MF : C₆H₆
MW : 78.11

SECTION 4: First aid measures

First Aid Measures

General advice

Immediate medical attention is required. In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

General advice	Immediate medical attention is required. In case of accident or unwellness, s				
	advice immediate	ly (show	directions for use or	safety data sheet	if possible).
Eye contact	Immediately flush	with plenty	of water. After initial	flushing, remove any	contact lenses.
	continue flushing	for at least	15 minutes. Keep	eye wide open	while rinsing. If
	persist, call a physician.				
Skin Contact	Wash off immediately	with	plenty of water.		
Inhalation	Remove to fresh	air Call a	physician If breathing	is irregular	or stopped, administer
	artificial respiration	Avoid direct	contact with skin. Use	barrier to give	mouth-to-mouth
Ingestion	Do NOT induce vomiting.		Rinse mouth. Drink plenty	of water. If symptoms	persist, call a physician.
	physician.				
Self-protection of the first aider	Remove all sources	of ignition.			

Eye contact

Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing. If symptoms persist, call a physician.

Skin Contact

Wash off immediately with plenty of water.

Inhalation

Remove to fresh air Call a physician If breathing is irregular or stopped, administer artificial respiration Avoid direct contact with skin. Use barrier to give mouth-to-mouth resuscitation

Ingestion

Do NOT induce vomiting. Rinse mouth. Drink plenty of water. If symptoms persist, call a physician.

Self-protection of the first aider

Remove all sources of ignition.

Most important symptoms and effects, both acute and delayed

Symptoms

No information available.

Indication of any immediate medical attention and special treatment needed

Note to physicians

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Suitable Extinguishing Media

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

Unsuitable Extinguishing Media

No information available.

Specific hazards arising from the chemical

Specific hazards arising from the chemical

No information available.

Hazardous combustion products

Carbon oxides.

Explosion data

Sensitivity to Mechanical Impact

No information available.

Sensitivity to Static Discharge

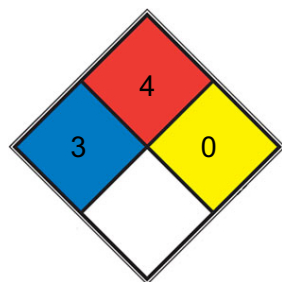
No information available.

Protective equipment and precautions for firefighters

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 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

Will rapidly or completely vaporize at normal atmospheric pressure and temperature, or is readily dispersed in air and will

☒ FIRE 4 burn readily. Includes pyrophoric substances. Flash point below room temperature at 22.8 °C (73 °F). (e.g. acetylene, propane, [hydrogen gas](#))

☒ 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, protective equipment and emergency procedures

Personal precautions

Remove all sources of ignition. Evacuate personnel to safe areas. Ensure adequate ventilation, especially in confined areas.

Environmental precautions

Environmental precautions

Prevent further leakage or spillage if safe to do so. Prevent product from entering drains.

See Section 12 for additional Ecological Information.

Methods and material for containment and cleaning up

Methods for containment

Prevent further leakage or spillage if safe to do so.

Methods for cleaning up

Pick up and transfer to properly labeled containers. Dam up. Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust).

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Ensure adequate ventilation, especially in confined areas. Keep away from heat, sparks, flame and other sources of ignition (i.e., pilot lights, electric motors and static electricity).

Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment. All equipment used when handling the product must be grounded.

Conditions for safe storage, including any incompatibilities

Storage Conditions

Keep tightly closed in a dry and cool place. Keep in properly labeled containers. Store at room temperature.

Incompatible materials

None known based on information supplied.

SECTION 8: Exposure controls/personal protection

Control parameters

Exposure Guidelines

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Other Information

Vacated limits revoked by the Court of Appeals decision in AFL-CIO v. OSHA, 965 F.2d 962 (11th Cir., 1992).

Column 1	Column 2	Column 3	Column 4
Pentane 109-66-0	TWA: 1000 ppm	TWA: 1000 ppm TWA: 2950 mg/m3 (vacated) TWA: 600 ppm (vacated) TWA: 1800 mg/m3 (vacated) STEL: 750 ppm (vacated) STEL: 2250 mg/m3	IDLH: 1500 ppm Ceiling: 610 ppm 15 min Ceiling: 1800 mg/m3 15 min TWA: 120 ppm TWA: 350 mg/m3

NIOSH IDLH Immediately Dangerous to Life or Health

Appropriate engineering controls

Engineering Controls

Showers

Eyewash stations

Ventilation systems

Individual protection measures, such as personal protective equipment

Eye/face protection

Tight sealing safety goggles.

Skin and Body Protection

Wear protective gloves and protective clothing.

Respiratory protection

If exposure limits are exceeded or irritation is experienced, NIOSH/MSHA approved respiratory protection should be worn. Positive-pressure supplied air respirators may be required for high airborne contaminant concentrations. Respiratory protection must be provided in accordance with current local regulations.

General Hygiene Considerations

When using do not eat, drink or smoke. Regular cleaning of equipment, work area and clothing is recommended.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State	liquid
Appearance	No information available
Odor	No information available
pH	No information available

Melting point/freezing point	No information available
Boiling point	88 °C
Flash point	-7 °C
Liquid Density	0.805 g/mL
Evaporation rate	No information available
Upper flammability limits	No information available
Lower flammability limit	No information available
Vapor pressure	No information available
Vapor density	No information available
Specific gravity	No information available
Water solubility	Immiscible with water.
Solubility in other solvents	No information available
Partition coefficient	No information available
Autoignition temperature	No information available
Decomposition temperature	No information available
Kinematic viscosity	No information available
Explosive properties	No information available
Oxidizing properties	No information available
Density and/or relative density	0,805 g/cm ³
Colour	Colorless to Yellow

SECTION 10: Stability and reactivity

Reactivity

Not applicable

Chemical stability

Stable under recommended storage conditions.

Possibility of Hazardous Reactions

None under normal processing.

Hazardous polymerization

No information available.

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong oxidizing agents.

Hazardous Decomposition Products

Carbon oxides.

SECTION 11: Toxicological information

Information on likely routes of exposure

Inhalation

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

Eye contact

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

Skin Contact

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

Ingestion

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

Information on toxicological effects

Symptoms

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

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Chronic Toxicity

Classified based on available data. For more details, see section 2. Target Organ Effects Central nervous system, Eyes, Respiratory system, Skin.

Numerical measures of toxicity - Product Information

Unknown acute toxicity

50% of the mixture consists of ingredient(s) of unknown toxicity

The following values are calculated based on chapter 3.1 of the GHS document

ATEmix (oral)

2000 mg/kg

ATEmix (dermal)

3000 mg/kg

ATEmix (inhalation-dust/mist)

364 mg/l

ATEmix (inhalation-vapor)

364 mg/l

SECTION 12: Ecological information

Ecotoxicity

Toxic to aquatic life with long lasting effects

Chemical name	Algae/aquatic plants	Fish	Toxicity to Microorganisms	Crustacea
				9.74: 48 h

Pentane 109-66-0	9.99: 96 h Lepomis macrochirus mg/L LC50 11.59: 96 h Pimephales promelas mg/L LC50 9.87: 96 h Oncorhynchus mykiss mg/L LC50	Daphnia magna mg/L EC50
109-66-0		

50% of the mixture consists of components(s) of unknown hazards to the aquatic environment.

Pentane -

9.99: 96 h Lepomis - 9.74: 48 h Daphnia magna

Persistence and degradability

No information available.

Bioaccumulation

No information available.

Mobility

No information available.

Pentane

3.39 109-66-0

SECTION 13: Disposal considerations

Disposal of wastes

Disposal should be in accordance with applicable regional, national and local laws and regulations.

Contaminated packaging

Do not reuse container.

Other Information

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

California Hazardous Waste Status

This product contains one or more substances that are listed with the State of California as a hazardous waste.

Chemical name	California Hazardous Waste Status
Pentane 109-66-0	Toxic Ignitable

Pentane

Toxic

SECTION 14: Transport information

DOT

UN/ID no

UN3295

Hazard Class

3

Packing Group

II

Proper shipping name

Hydrocarbons, liquid, n.o.s.

Description

UN3295, Hydrocarbons, liquid, n.o.s., 3, II

Emergency Response Guide Number

128

IMDG**UN/ID no**

UN3295

Hazard Class

3

Packing Group

II

Proper shipping name

Hydrocarbons, liquid, n.o.s.

Description

UN3295, Hydrocarbons, liquid, n.o.s. (Pentane), 3, II, (-7°C c.c.), Marine pollutant

EmS-No

F-E, S-D

IATA**UN/ID no**

UN3295

Hazard Class

3

Packing Group

II

Proper shipping name

Hydrocarbons, liquid, n.o.s.

Description

UN3295, Hydrocarbons, liquid, n.o.s., 3, II

ERG Code

3H

SECTION 15: Regulatory information

International Inventories

All of the components in the product are on the following Inventory lists

TSCA (United States): Canada (DSL/NDL) Europe (EINECS/ELINCS/NLP) South Korea (KECL):

X - Listed

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

EINECS/ELINCS - European Inventory of Existing Chemical Substances/European List of Notified Chemical Substances

ENCS - Japan Existing and New Chemical Substances

IECSC - China Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

Chemical name	TSCA	DSL	NDL	EINECS	ELINCS	ENCS	IECSC	KECL	PICCS	AICS
Pentane	X	X	-	X	-	X	X	X	X	X
1,5-Hexadiyne	X	-	X	X	-	-	-	X	-	-

US Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

SARA 311/312 Hazard Categories

Acute health hazard

Yes

Chronic Health Hazard

No

Fire hazard

Yes

Sudden release of pressure hazard

No

Reactive hazard

No

CWA (Clean Water Act)

This product does not contain any substances regulated as pollutants pursuant to the Clean Water Act (40 CFR 122.21 and 40 CFR 122.42).

US State Regulations

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Chemical name	New Jersey	Massachusetts	Pennsylvania

Pentane 109-66-0	X	X	X
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SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.