

Chemical Safety Data Sheet MSDS / SDS

2,4-HEPTADIEN-6-ONE

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

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

Product name : 2,4-HEPTADIEN-6-ONE
CBnumber : CB6719647
CAS : 3916-64-1
Synonyms : 3,5-Heptadien-2-one,heptadienone

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

P271 Use only outdoors or in a well-ventilated area.
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.
P312 Call a POISON CENTER or doctor/physician if you feel unwell.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P501 Dispose of contents/container to.....
P363 Wash contaminated clothing before reuse.
P322 Specific measures (see ...on this label).
P312 Call a POISON CENTER or doctor/physician if you feel unwell.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P501 Dispose of contents/container to.....

P330 Rinse mouth.

P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

Hazard statements

H312 Harmful in contact with skin

H302 Harmful if swallowed

H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2,4-HEPTADIEN-6-ONE
Synonyms	: 3,5-Heptadien-2-one,heptadienone
CAS	: 3916-64-1
MF	: C7H10O
MW	: 110.15

SECTION 4: First aid measures

If inhaled

Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER or doctor/ physician if you feel unwell.

In case of skin contact

Take off all contaminated clothing immediately. If on skin, rinse well with water. If skin irritation or rash occurs: Get medical advice/ attention.

In case of eye contact

Rinse with plenty of water. If easy to do, remove contact lens, if worn. If eye irritation persists: Get medical advice/ attention.

If swallowed

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

Most important symptoms and

None known. effects, both acute and delayed

SECTION 5: Firefighting measures

Suitable extinguishing media

Dry powder, Foam, Water spray, Carbon dioxide (CO2)

Specific hazards during fire fighting

No information available.

Specific extinguishing methods

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Immediately evacuate personnel to safe areas. Cool closed containers exposed to fire with water spray. Remove undamaged containers from fire area if it is safe to do so.

Special protective equipment for fire-fighters

Use personal protective equipment.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear suitable protective equipment. Keep people away from and upwind of spill/leak. Ensure adequate ventilation. Entry to non-involved personnel should be controlled around the leakage area by roping off, etc.

Environmental precautions

Prevent product from entering drains.

Methods and materials for containment and cleaning up

Collect as much of the spill as possible with a suitable absorbent material.

SECTION 7: Handling and storage

Handling

Technical measures

Prevent generation of vapor or mist. Take precautionary measures against static discharge. Use explosion-proof equipment.

Local/Total ventilation

Ensure adequate ventilation. Use a local exhaust ventilation.

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wear personal protective equipment. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Do not subject to grinding, shock or friction. Wash hands and face thoroughly after handling.

Avoidance of contact

Oxidizing agents

Storage

Conditions for safe storage

Keep container tightly closed. Store in a cool and shaded area. Keep in a well-ventilated place. Use explosion-proof equipment.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Components	CAS RN	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
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Hydroquinone	123-31-9	PC-TWA	1 mg/m ³	CN OEL
		PC-STEL	2 mg/m ³	CN OEL
		TWA	1 mg/m ³	ACGIH

Components CAS RN Value type Control parameters Basis (Form of ex- / Permissible conposure) centration

Hydroquinone 123-31-9 PC-TWA 1 mg/m³ CN OEL

PC-STEL 2 mg/m³ CN OEL

TWA 1 mg/m³ ACGIH

Engineering measures

Install a closed system or local exhaust.

Also install safety shower and eye bath.

Personal protective equipment

Respiratory protection

Gas mask

Eye/face protection

Safety glasses

Face-shield

Skin and body protection

Protective suit

Hand protection

Protective gloves *Use personal protective equipment(PPE) approved under appropriate government standards and follow local and national regulations.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

white - yellow

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/freezing point

No data available

Boiling point/boiling range

88 °C (39 hPa)

Flash point

56 °C (Calculated value)

Evaporation rate

No data available

Flammability

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 density

0.90

Solubility(ies)**Water solubility**

No data available

Solubility in other solvents

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity**Viscosity, dynamic**

No data available

Viscosity, kinematic

No data available

Molecular weight

110.16 g/mol

Physical state

clear liquid

SECTION 10: Stability and reactivity**Reactivity**

No data available

Chemical stability

Polymerization may occur under the influences of heat, light or on contact with polymerization initiators such as peroxides etc.

Possibility of hazardous reactions

None under normal processing.

Conditions to avoid

Heat. Electrical spark Open flame Electrostatic discharge Exposure to light.

Incompatible materials

Oxidizing agents

Hazardous decomposition products

Carbon monoxide, Carbon dioxide (CO₂)

SECTION 11: Toxicological information**Acute toxicity****Product****Acute oral toxicity**

Assessment: The component/mixture is moderately toxic after single ingestion.

Acute inhalation toxicity

Assessment: The component/mixture is moderately toxic after short term inhalation.

Acute dermal toxicity

Assessment: The component/mixture is moderately toxic after single contact with skin.

Components

2,4-Heptadien-6-one

Acute oral toxicity

LD50 (Rat): 1,210 mg/kg Assessment: The component/mixture is moderately toxic after single ingestion.

Acute inhalation toxicity

Assessment: The component/mixture is moderately toxic after short term inhalation.

Acute dermal toxicity

Assessment: The component/mixture is moderately toxic after single contact with skin.

Hydroquinone

Acute oral toxicity

LDLo (Humans): 29 mg/kg Assessment: The component/mixture is moderately toxic after single ingestion.

LD50 (Rat)

302 mg/kg

Acute dermal toxicity

LD50 (Rabbit): > 2,000 mg/kg Assessment: The substance or mixture has no acute dermal toxicity

Acute toxicity (other routes of administration)

LD50 (Rat): 170 mg/kg Application Route: Intraperitoneal injection

Skin corrosion/irritation

Components

Hydroquinone

Result

Skin irritation

Serious eye damage/eye irritation

Components

Hydroquinone

Result

Irreversible effects on the eye

Respiratory or skin sensitization

Components

Hydroquinone

Assessment

May cause sensitization by skin contact.

Germ cell mutagenicity

Components

Hydroquinone

Germ cell mutagenicity - Assessment

Presumed to induce heritable mutations in the germ cells of humans.

Carcinogenicity

Components

Hydroquinone

Carcinogenicity - Assessment

Suspected human carcinogens

Reproductive toxicity

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

STOT-single exposure

Components

Hydroquinone

Target Organs

Kidney, Central nervous system

Assessment

Causes damage to organs.

STOT-repeated exposure

Components

Hydroquinone

Target Organs

Blood, Respiratory system

Assessment

Causes damage to organs through prolonged or repeated exposure.

Target Organs

Liver, Kidney, Central nervous system

Assessment

May cause damage to organs through prolonged or repeated exposure.

Repeated dose toxicity

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

Aspiration toxicity

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

RTECS No.

MI5495000 (2,4-Heptadien-6-one) MX3500000 (Hydroquinone)

SECTION 12: Ecological information

Ecotoxicity

Components:

Hydroquinone:

Toxicity to fish

LC50 (Oncorhynchus mykiss (rainbow trout)): 0.044 mg/l Exposure time: 96 h

Toxicity to daphnia and other aquatic invertebrates

EC50 (Daphnia magna (Water flea)): 0.061 mg/l Exposure time: 48 h

Toxicity to algae/aquatic plants

EC50 (Selenastrum capricornutum (green algae)): 0.053 mg/l Exposure time: 72 h

Ecotoxicology Assessment

Acute aquatic toxicity

Very toxic to aquatic life.

Chronic aquatic toxicity

Very toxic to aquatic life with long lasting effects.

Persistence and degradability

No data available

Bioaccumulative potential

Components:**Hydroquinone:**

octanol/water

Partition coefficient: octanol/water

0.59

Mobility in soil**Components:****Hydroquinone:**

tal compartments

Distribution among environmental compartments

Koc: 240

Other adverse effects

No data available

SECTION 13: Disposal considerations

Disposal methods**Waste from residues**

Disposal in accordance with local and national regulations. Take precautions against ignition or explode. Entrust disposal to a licensed waste disposal company.

Contaminated packaging

Disposal in accordance with local and national regulations. Before disposal of used container, remove contents completely.

SECTION 14: Transport information

International Regulations**Domestic regulation**

SECTION 15: Regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration**Registration/Notification number**

B1A232216104

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.

The ingredients of this product are reported in the following inventories

CH BAGREG

Not in compliance with the inventory

TSCA

Substance(s) not listed on TSCA inventory

AICS

Not in compliance with the inventory

DSL

This product contains the following components that are not on the Canadian DSL nor NDSL.

2,4-Heptadien-6-one

ENCS

Not in compliance with the inventory

ISHL

Not in compliance with the inventory

KECI

Not in compliance with the inventory

PICCS

On the inventory, or in compliance with the inventory

IECSC

Not in compliance with the inventory

NZIoC

Not in compliance with the inventory

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.