

Safety Data Sheet

according to 1907/2006/EC, Article 31

Printing date: 12.11.2007

Revision: 12.11.2007

1 Identification of substance:

- **Product details:**
- **Trade name:** **Isophorone**
- **Application of the substance / the preparation** Chemicals for synthesis
- **Supplier/Manufacturer:**
Penpet Petrochemical Trading GmbH
Merkur-Park
Sieker Landstrasse 126
22143 Hamburg
Germany
Tel: +49 40 675 799 0
Fax: +49 40 675 799 99 / 88
- **Email competent person:** angelika.torges@kft.de
- **Information department:** See supplier/manufacturer
- **Emergency information:** National Poisons Information Centre Tel.: +44 (0)870 6006266

2 Hazards identification

- **Hazard description:**



Carc. Cat. 3
Xn Harmful

- **Information pertaining to particular dangers for man and environment:**
Under working conditions mainly resorbed via respiratory tract.
R 21/22 Harmful in contact with skin and if swallowed.
R 36/37 Irritating to eyes and respiratory system.
R 40 Limited evidence of a carcinogenic effect.
- **Classification system:**
The classification was made according to the latest editions of the EU-lists, and expanded using company data and specialized literature.

3 Composition/information on ingredients

- **Chemical characterization:**
- **CAS No. Description:**
78-59-1 3,5,5-trimethylcyclohex-2-enone
- **Identification number(s):**
- **EINECS Number:** 201-126-0
- **EU Number:** 606-012-00-8

4 First aid measures

- **General information:**
First aid personnel should pay attention to their own safety.
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may occur even after several hours; therefore medical observation is suggested for at least 48 hours after the accident.
- **After inhalation:**
Remove victim from contaminated area. If breathing is difficult, give oxygen. If breathing stops, provide artificial respiration. Call a doctor.
In case of unconsciousness, place patients on their side in a stable position for transportation.

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· After skin contact:

Remove soiled clothes and shoes.

Clean effected skin thoroughly with water and a mild cleansing agent. No residues shall remain on the skin.

If available apply polyethylenglycol (PEG 400, Lutrol) and let it remain on the skin for several minutes.

Afterwards:

Wash with water.

Seek medical treatment.

· After eye contact:

Rinse the eyes with open eyelids for 10 - 15 minutes with water. Then consult a doctor or better an eye specialist.

· After swallowing:

Rinse out mouth and then drink plenty of water.

Never give anything by mouth to a unconscious person.

Do not administer milk or alcohol.

Do not administer edible oils or ricinus oil.

Do not induce vomiting.

If vomitting occurs spontaneously:

Hold the head of the casualty low with the body in a prone position in order to avoid aspiration.

Call for a doctor immediately.

· Information for doctor:**· The following symptoms may occur:**

Local irritation symptoms

Disturbance of central nervous system

· Danger:

If swallowed or in case of vomiting, danger of entering the lungs.

Danger of pneumonia.

· Treatment:

Symptomatic treatment

(decontamination, vital functions)

In cases of irritation to the lungs, initial treatment with Dexametason metered aerosol.

Monitor circulation

Acid-base-balance should be controlled.

Monitoring of liver- and renal functions.

No specific antidote known.

5 Fire fighting measures

· Suitable extinguishing agents:

Fire-extinguishing powder

Carbon dioxide (CO₂)

Use fire fighting measures that suit the environment.

· Special hazards caused by the material, its products of combustion or resulting gases:

Dangerous decomposition product see chapter 10: stability and reactivity

· Protective equipment:

Wear self-contained respiratory protective device.

Wear fully protective suit.

Rubber and plastic clothing will be attacked under prolonged action.

· Additional information:

Heating leads to pressure increase entailing danger of bursting and explosion. Immediately cool neighbouring packages and containers with sprayed water and, if possible, remove them out of the danger zone

Dispose of fire debris and contaminated fire fighting water in accordance with official regulations.

Collect contaminated fire fighting water separately. It must not enter the sewage system.

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6 Accidental release measures

- **Person-related safety precautions:**



Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Use respiratory protective device against the effects of fumes/dust/aerosol.

Avoid contact with eyes and skin.

- **Measures for environmental protection:**

Do not allow product to reach sewage system or any water course.

Do not allow to penetrate the ground/soil.

- **Measures for cleaning/collecting:**

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Ensure adequate ventilation.

Send for recovery or disposal in suitable receptacles.

Dispose contaminated material as waste according to item 13.

- **Additional information:** See Section 8 for information on personal protection equipment.

7 Handling and storage

- **Handling**

- **Information for safe handling:**

Ensure good ventilation/exhaustion at the workplace.

Ensure good interior ventilation, especially at floor level. (Fumes are heavier than air).

Keep away from heat and direct sunlight.

Keep receptacles tightly sealed.

Use solvent-proof equipment.

Restrict the quantity stored at the work place.

Keep the working area dry and clean.

Avoid contact with eyes and skin.

Avoid inhalation of vapours.

- **Information about protection against explosions and fires:**



Keep ignition sources away - Do not smoke.

Fumes can combine with air to form an explosive mixture.

- **Storage**

- **Requirements to be met by storerooms and receptacles:**

Observe national regulations for storage of flammable liquids.

Store container tightly sealed at a cool and dry place with sufficient ventilation.

Provide solvent resistant, sealed floor.

Suitable material:

Steel

Copper

- **Information about storage in one common storage facility:**

Store away from foodstuffs.

Store away from feed.

Follow regulations for flammable liquids.

- **Further information about storage conditions:**

Keep receptacle tightly sealed.

Protect from heat and direct sunlight.

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- **Storage class** 3B Flammable Liquids

8 Exposure controls and personal protection

- **Additional information about design of technical systems:** No further data; see item 7.

- **Components with limit values that require monitoring at the workplace:**

78-59-1 3,5,5-trimethylcyclohex-2-enone

WEL (Great Britain) Short-term value: 29 mg/m³, 5 ppm

- **Additional information:** The lists that were valid during the creation were used as basis.

- **Personal protective equipment**

- **General protective and hygienic measures:**

Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing
Wash hands before breaks and at the end of work.
Avoid contact with the eyes and skin.
Do not inhale gases / fumes / aerosols.
Do not eat or drink while working.
Provide eye bath.

- **Breathing equipment:**

Not necessary if room is well-ventilated.
In case of unintentional release of the substance, exceeding the occupational exposure limit value:



In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

Short term filter device:

Filter A

- **Protection of hands:**

Chemical resistant gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
After use of gloves apply skin-cleaning agents and skin cosmetics.

- **Material of gloves:**

Butyl rubber, BR

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

- **Penetration time of glove material:**

The exact break-through time has to be found out by the manufacturer of the protective gloves and has to be observed.

- **As protection from splashes gloves made of the following materials are suitable:** Nitrile rubber, NBR

- **Eye protection:**

Safety glasses

If vapours or aerosols arise which may injure the eyes ,
wearing of a full mask is recommended.

- **Body protection:**

Solvent resistant protective clothing

Flame retarding protective clothing

According to hazard:

Apron

Boots

Use protective suit.

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9 Physical and chemical properties:

· General Information

Form: Fluid
Colour: Clear
Odour: like peppermint

· Change in condition:

Melting point/Melting range: -8.1°C
Boiling point/Boiling range: 215°C

· **Flash point:** 96°C

· **Ignition temperature:** 460°C

· **Danger of explosion:** Product is not explosive. However, formation of explosive air/vapour mixtures are possible.

· Explosion limits:

Lower: 0.8 Vol %
Upper: 3.8 Vol %

· **Vapour pressure at 20°C:** 0.33 hPa

· **Density at 20°C:** 0.92 g/cm³

· Solubility in / Miscibility with

Water at 20°C: 12 g/l

· **Segregation coefficient (n-octanol/water):** 1.66 log POW

10 Stability and reactivity

· **Thermal decomposition / conditions to be avoided:** No decomposition if used and stored according to specifications.

· **Dangerous reactions:** No dangerous reactions known

· Dangerous products of decomposition:

In the case of fire or at high temperatures the formation of the following decomposition products is possible.

11 Toxicological information

· Acute toxicity:

· LD/LC50 values that are relevant for classification:

Oral LD₅₀ 1500 mg/kg (rabbit)

Dermal LD₅₀ 1500 mg/kg (rabbit)

· Primary irritant effect:

· on the skin:

No irritating effect.

Risk of absorption

· on the eye: Irritating effect.

· **Sensitization:** No sensitizing effects known.

· Other information (about experimental toxicology):

Ames-test: no mutagenic effects

Mutagenicity (mammalian cell test): chromosomes aberration negative

· Additional toxicological information:

After swallowing: irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

· CMR effects (carcinogenity, mutagenicity and toxicity for reproduction)

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12 Ecological information

- **Information about elimination (persistence and degradability):**
- **Other information:** The product is readily biodegradable.
- **Behaviour in environmental systems:**
- **Mobility and bioaccumulation potential:** Slight bioaccumulation possible.
- **Ecotoxicological effects:**
- **Aquatic toxicity:**

EC₅₀/24h 254 mg/l (daphnia magna)IC₅₀/72h 475 mg/l (des)LC₅₀/48h 209 mg/l (leuciscus idus)

- **General notes:**

Water hazard class 1 (German Regulation) (Self-assessment): slightly hazardous for water.

According to appendix 3 of VwVwS dated 17.05.1999 (German regulation)

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

13 Disposal considerations

- **Product:**
- **Recommendation:**



Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

Disposal according to instructions of local authorities.

- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- **Land transport ADR/RID (cross-border)**
- **ADR/RID class:** -
No hazardous good according to the regulation.
- **Maritime transport IMDG:**
- **IMDG Class:** -
No hazardous good according to the regulation.
- **Air transport ICAO-TI and IATA-DGR:**
- **ICAO/IATA Class:** -
No hazardous good according to the regulation.

15 Regulations

- **Markings according to EC guidelines:**
The product has been classified and marked in accordance with EU Directives / Ordinance on Hazardous Materials "EC-labelling"
- **Code letter and hazard designation of product:**

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- **Risk phrases:**
21/22 Harmful in contact with skin and if swallowed.
36/37 Irritating to eyes and respiratory system.

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40 Limited evidence of a carcinogenic effect.

Safety phrases:

- 13 Keep away from food, drink and animal feedingstuffs.
- 23 Do not breathe fumes/aerosol.
- 36/37/39 Wear suitable protective clothing, gloves and eye/face protection.
- 46 If swallowed, seek medical advice immediately and show this container or label.

National regulations
Information about limitation of use:

- Restrictions on juvenile employment must be observed.
- Employment restrictions concerning pregnant and lactating women must be observed.

Technical guidance (air):
Class Share in %

- I 100.0

- **Water hazard class:** Water hazard class 1 (Self-assessment): slightly hazardous for water.

16 Other information:

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

Department issuing MSDS:

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Sources:

RTECS database
 NTP (National Toxicological Program)