

MATERIAL SAFETY DATA SHEET

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Version 1.4

Section 1 - Product and Company Information

Product Name ISOPHORONE, 97%
Product Number I18709
Brand ALDRICH

Company Sigma-Aldrich
Address 3050 Spruce Street
SAINT LOUIS MO 63103 US

Technical Phone: 800-325-5832
Fax: 800-325-5052
Emergency Phone: 314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
ISOPHORONE	78-59-1	No

Formula C9H14O
Synonyms Isoacetophorone * Isoforon * Isoforone (Italian)
* Isophoron * Isophorone (ACGIH:OSHA) * Izoforon
(Polish) * NCI-C55618 *
1,1,3-Trimethyl-3-cyclohexene-5-one *
3,3,5-Trimethyl-5-cyclohexen-1-one *
3,5,5-Trimethyl-2-cyclohexene-1-one *
3,5,5-Trimethyl-2-cyclohexen-1-on (German, Dutch)
* 3,5,5-Trimethylcyclohex-2-ene-1-one *
3,5,5-Trimetil-2-cicloesen-1-one (Italian)

RTECS Number: GW7700000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Harmful.

Harmful in contact with skin and if swallowed. Irritating to respiratory system. Limited evidence of a carcinogenic effect.

Risk of serious damage to eyes.

Possible Carcinogen (US). Target organ(s): Lungs. Liver. Kidneys.

HMIS RATING

HEALTH: 2*

FLAMMABILITY: 1

REACTIVITY: 0

NFPA RATING

HEALTH: 2

FLAMMABILITY: 1

REACTIVITY: 0

*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician immediately.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

FLASH POINT

204.8 °F 96 °C Method: closed cup

EXPLOSION LIMITS

Lower: 0.8 % Upper: 3.8 %

AUTOIGNITION TEMP

462 °C

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves. Wear disposable coveralls and discard them after use.

METHODS FOR CLEANING UP

Cover with dry lime or soda ash, pick up, keep in a closed container, and hold for waste disposal. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe dust. Do not get in eyes, on skin,

Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	204.8 °F 96 °C	Method: closed cup
Explosion Limits	Lower: 0.8 % Upper: 3.8 %	
Flammability	N/A	
Autoignition Temp	462 °C	
Refractive Index	1.478	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.

Materials to Avoid: Strong oxidizing agents, Strong acids, Strong bases.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.

Skin Absorption: Harmful if absorbed through skin.

Eye Contact: Causes severe eye irritation.

Inhalation: May be harmful if inhaled. Vapor or mist is irritating to the mucous membranes and upper respiratory tract.

Ingestion: Harmful if swallowed.

TARGET ORGAN(S) OR SYSTEM(S)

Central nervous system. Lungs. Liver. Kidneys.

SIGNS AND SYMPTOMS OF EXPOSURE

CNS depression. Exposure can cause: Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. Narcotic effect.

TOXICITY DATA

Oral

Rat

1870 mg/kg

LD50

Inhalation

Rat

7,000 mg/m³

LC50

Remarks: Behavioral: Somnolence (general depressed activity).

Skin and Appendages: Other: Hair. Lungs, Thorax, or

Respiration:Dyspnea.

Skin
Rat
1390 mg/kg
LD50

Oral
Mouse
2690 mg/kg
LD50

Oral
Rabbit
1420 mg/kg
LD50

Skin
Rabbit
1500 UL/KG
LD50

Oral
Guinea pig
700 mg/kg
LD50

Inhalation
Guinea pig
4,600 ppm
LC50

IRRITATION DATA

Eyes
Human
25 ppm
15M

Skin
Rabbit
100 mg
24H
Remarks: Mild irritation effect

Eyes
Rabbit
0.92 mg
Remarks: Severe irritation effect

Eyes
Rabbit
100 mg
24H
Remarks: Moderate irritation effect

Eyes
Guinea pig
840 ppm
4H
Remarks: Severe irritation effect

CHRONIC EXPOSURE - CARCINOGEN

Result: This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

Species: Rat

Route of Application: Oral

Dose: 180 GM/KG

Exposure Time: 2Y

Frequency: I

Result: Kidney, Ureter, Bladder:Tumors. Tumorigenic:Equivocal tumorigenic agent by RTECS criteria.

Species: Mouse

Route of Application: Oral

Dose: 258 GM/KG

Exposure Time: 2Y

Frequency: I

Result: Kidney, Ureter, Bladder:Kidney tumors. Tumorigenic:Carcinogenic by RTECS criteria.

NTP CARCINOGEN LIST

Rating: Some evidence.

Species: Rat

Route: Gavage

ACGIH CARCINOGEN LIST

Result: CONFIRMED ANIMAL CARCINOGEN

CHRONIC EXPOSURE - MUTAGEN

Species: Rat

Dose: 5 MMOL/L

Cell Type: liver

Mutation test: Unscheduled DNA synthesis

Species: Mouse

Dose: 400 MG/L

Cell Type: lymphocyte

Mutation test: Mutation in mammalian somatic cells.

Species: Hamster

Dose: 1250 MG/L

Cell Type: lung

Mutation test: Cytogenetic analysis

Species: Hamster

Dose: 1 GM/L

Cell Type: ovary

Mutation test: Sister chromatid exchange

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible

solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations. (DN)Requires special label: "Contains a substance which is regulated by Dannish work environmental law due to the risk of carcinogenic properties."

Section 14 - Transport Information

DOT

Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU DIRECTIVES CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 21/22-36/37-40
Risk Statements: Harmful in contact with skin and if swallowed. Irritating to eyes and respiratory system. Limited evidence of a carcinogenic effect.
S: 13-23-36/37/39-46
Safety Statements: Keep away from food, drink, and animal feedingstuffs. Do not breathe vapor. Wear suitable protective clothing, gloves, and eye/face protection. If swallowed, seek medical advice immediately and show this container or label.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Harmful.
Risk Statements: Harmful in contact with skin and if swallowed. Irritating to respiratory system. Limited evidence of a carcinogenic effect. Risk of serious damage to eyes.
Safety Statements: Keep away from food, drink, and animal feedingstuffs. Do not breathe vapor. Wear suitable protective clothing, gloves, and eye/face protection. If swallowed, seek medical advice immediately and show this container or label.
US Statements: Possible Carcinogen (US). Target organ(s): Lungs. Liver. Kidneys.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not

purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.