

## Material Safety Data Sheet

Date Printed: 16/DEC/2004

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Version 1.7

According to 91/155/EEC

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1 - Product and Company Information

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Product Name ISOPHORONE  
Product Number 59190  
  
Company Sigma-Aldrich Pte Ltd  
#08-01 Citilink Warehouse  
Singapore 118529  
Singapore  
Technical Phone # 65 271 1089  
Fax 65 271 1571

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2 - Composition/Information on Ingredients

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Product Name	CAS #	EC no	Annex I Index Number
ISOPHORONE	78-59-1	201-126-0	606-012-00-8

Formula C9H14O  
Molecular Weight 138.21 AMU  
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)

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3 - Hazards Identification

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## SPECIAL INDICATION OF HAZARDS TO HUMANS AND THE ENVIRONMENT

Harmful in contact with skin and if swallowed. Irritating to eyes and respiratory system. Limited evidence of a carcinogenic effect. Carc. Cat.3

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4 - First Aid Measures

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## AFTER INHALATION

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

## AFTER SKIN CONTACT

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

## AFTER EYE CONTACT

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.

AFTER INGESTION

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

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5 - Fire Fighting Measures

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EXTINGUISHING MEDIA

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

SPECIAL RISKS

Specific Hazard(s): Emits toxic fumes under fire conditions.

SPECIAL PROTECTIVE EQUIPMENT FOR FIREFIGHTERS

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

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6 - Accidental Release Measures

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PERSONAL PRECAUTION PROCEDURES 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.

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7 - Handling and Storage

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HANDLING

Directions for Safe Handling: Do not breathe dust. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE

Conditions of Storage: Keep tightly closed.

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8 - Exposure Controls / Personal Protection

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ENGINEERING CONTROLS

Use only in a chemical fume hood. Safety shower and eye bath.

GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Wash thoroughly after handling.

EXPOSURE LIMITS

Country	Source	Type	Value
Poland		NDS	5 MG/M3
Poland		NDSch	10
Poland		NDSP	-

EXPOSURE LIMITS - DENMARK

Source	Type	Value
OEL	TWA	25 mg/m3
		5 ppm

Remarks: L

## EXPOSURE LIMITS - GERMANY

Source	Type	Value
TRGS 900	OEL	11 mg/m3 2 ppm

Remarks: =1=

## EXPOSURE LIMITS - NORWAY

Source	Type	Value
	OEL	25 mg/m3 5 ppm

Remarks: T

## EXPOSURE LIMITS - SWEDEN

Source	Type	Value
	CLV (Ceili	30 mg/m3 5 ppm

## EXPOSURE LIMITS - SWITZERLAND

Source	Type	Value
OEL	OEL	11 mg/m3 2 ppm

Remarks: C

## EXPOSURE LIMITS - UNITED KINGDOM

Source	Type	Value
OEL	STEL	29 mg/m3 5 ppm

## PERSONAL PROTECTIVE EQUIPMENT

Respiratory Protection: Government approved respirator.

Hand Protection: Compatible chemical-resistant gloves.

Eye Protection: Chemical safety goggles.

## 9 - Physical and Chemical Properties

Appearance	Physical State: Clear liquid Color: Very faintly yellow-green	
Property	Value	At Temperature or Pressure
pH	N/A	
BP/BP Range	211 - 215 °C	
MP/MP Range	-8 °C	
Flash Point	96 °C	Method: closed cup
Flammability	N/A	
Autoignition Temp	462 °C	
Oxidizing Properties	N/A	
Explosive Properties	N/A	
Explosion Limits	Lower: 0.8 % Upper: 3.8 %	
Vapor Pressure	0.2 mmHg	20 °C
SG/Density	0.921 g/cm3	
Partition Coefficient	N/A	
Viscosity	N/A	
Vapor Density	4.77 g/l	
Saturated Vapor Conc.	N/A	
Evaporation Rate	N/A	
Bulk Density	N/A	
Decomposition Temp.	N/A	
Solvent Content	N/A	
Water Content	N/A	

Surface Tension	N/A
Conductivity	N/A
Miscellaneous Data	N/A
Solubility	N/A

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## 10 - Stability and Reactivity

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### 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

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## 11 - Toxicological Information

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RTECS NUMBER: GW7700000

### ACUTE TOXICITY

LD50  
Oral  
Rat  
1870 mg/kg

LC50  
Inhalation  
Rat  
7,000 mg/m3  
Remarks: Behavioral:Somnolence (general depressed activity).  
Lungs, Thorax, or Respiration:Dyspnea. Skin and Appendages:  
Other: Hair.

LD50  
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

LC50  
Inhalation  
Guinea pig  
4,600 ppm  
8H

#### 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

#### SIGNS AND SYMPTOMS OF EXPOSURE

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

#### 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 INFORMATION

Lungs. Central nervous system. Liver. Kidneys.

#### 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.

Rat  
Route of Application: Oral  
Exposure Time: 2Y  
Result: Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Kidney, Ureter, Bladder: Tumors.

Mouse  
Route of Application: Oral  
Exposure Time: 2Y  
Result: Tumorigenic: Carcinogenic by RTECS criteria. Kidney,  
Ureter, Bladder: Kidney tumors.

CHRONIC EXPOSURE - MUTAGEN

Rat  
5 MMOL/L  
Cell Type: liver  
Unscheduled DNA synthesis

Mouse  
400 MG/L  
Cell Type: lymphocyte  
Mutation in mammalian somatic cells.

Hamster  
1250 MG/L  
Cell Type: lung  
Cytogenetic analysis

Hamster  
1 GM/L  
Cell Type: ovary  
Sister chromatid exchange

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12 - Ecological Information

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No data available.

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13 - Disposal Considerations

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SUBSTANCE DISPOSAL

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.

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14 - Transport Information

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RID/ADR

Non-hazardous for road transport.

IMDG

Non-hazardous for sea transport.

IATA

Non-hazardous for air transport.

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15 - Regulatory Information

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CLASSIFICATION AND LABELING ACCORDING TO EU DIRECTIVES

ANNEX I INDEX NUMBER: 606-012-00-8

INDICATION OF DANGER: Xn

Harmful.

R-PHRASES: 21/22 36/37 40

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

effect.

S-PHRASES: 13 23 36/37/39 46

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.

#### COUNTRY SPECIFIC INFORMATION

Germany

WGK: 1

SWITZERLAND

SWISS POISON CLASS: 4

NORWAY

Labelling for organic solvents where the package is 1 liter or more.

YL-tall m3/l: 11040

YL-group: 5

Risk phrases: 20

Harmful by inhalation.

Safety phrases: 38 42 210

In case of insufficient ventilation, wear suitable respiratory equipment. During fumigation/spraying wear suitable respiratory equipment. Use compressed air- or fresh air line breathing apparatus in confined spaces.

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#### 16 - Other Information

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#### 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 2004 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.

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