

Safety data sheet as per Commission Regulation (EU) 2015/830

Product: Isophorone



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

1.1 Product identifier

Trade name	Isophorone
Chemical Name	3,5,5-trimethylcyclohex-2-enone
CAS Number	78-59-1
EC Number	201-126-0
Pre-Registration number (REACH)	05-2114672544-43-0000

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses	Solvent in printing inks, paints, lacquers, adhesives, copolymers, coatings, finishings and pesticides. Ingredient in wood preservatives and floor sealants Chemical intermediate
Uses identified against	Should not be used as part of cosmetic product

1.3 Details of the supplier of the safety data sheet:

Manufacturer	Prasol Chemicals Pvt. Ltd., Prasol House, Plot No.A-17/2/3, T.T.C. Indl. Area, Khairme M.I.D.C., Navi Mumbai - 400 710. Maharashtra, India.
Telephone	+91-22-27782555
Telefax	+91-22-27782430
e-mail address	sales@prasolchem.com; inquiry@prasolchem.com

1.4 Emergency telephone number

Telephone	+91-22- 27782555
Language	English

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Acute Toxicity (Oral)	Category 4	H302	Harmful if swallowed
Acute Toxicity (Dermal)	Category 4	H312	Harmful in contact with skin
Eye Irritation	Category 2	H319	Causes serious eye irritation
Carcinogenicity	Category 2	H351	Suspected of causing cancer
Specific Target Organ Toxicity	Category 3	H335	May cause respiratory irritation

Information concerning particular hazards for human and environment: No further information

2.2 Label elements

Labeling according to Regulation (EC) No 1272/2008 (CLP)

Hazard pictograms



GHS07

GHS08

Signal word Warning

Hazard statements

H302

Harmful if swallowed.

H312

Harmful in contact with skin.

H319

Causes serious eye irritation.

H335

May cause respiratory irritation.

H351

Suspected of causing cancer.

Precautionary statements

General P103

Read label before use.

Prevention P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P210

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P264

Wash hands thoroughly after handling.

P270

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

P280

Use protective gloves and eye protection.

Response

P302+P352

IF ON SKIN: Wash with plenty of water.

P305+P351+P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing



	P308+P313	IF exposed or concerned: Get medical attention.
	P312	Call a doctor if you feel unwell.
	P321	Specific treatment: wash with plenty of water.
	P337+P313	If eye irritation persists: Get medical attention
	P362+P364	Take off contaminated clothing and wash it before reuse.
	P370+P378	In case of fire: Use CO ₂ , dry powder, foam or water spray to extinguish
Storage	P403	Store in a well-ventilated area.
	P405	Store locked up.
Disposal	P501	Dispose of contents and container in accordance with national regulations

2.3 Other hazards

Not a PBT, vPVB substance according to the criteria of REACH regulation

SECTION 3: Composition/information on ingredients

3.1 Substances

Ingredient	CAS No.	EC No.	Concentration (%)
3,5,5-trimethylcyclohex-2-enone (isophorone)	78-59-1	201-126-0	98.5 min
3,5,5-trimethylcyclohex-3-en-1-one	471-01-2	207-434-1	1.5 max

Additional information:

Molecular Formula	C ₉ H ₁₄ O
Molecular Weight	138.21

SECTION 4: First aid measures

4.1 Description of first aid measures

General information

After inhalation

Take off all contaminated clothing immediately.

If inhaled, remove to fresh air. If breathing is difficult, give oxygen. If unconscious, evaluate the need for artificial respiration. Get immediate medical attention

After skin contact

Wash off with plenty of water immediately, seek medical advice if necessary.

After eye contact

Rinse with plenty of water immediately and seek medical advice.

After swallowing

Do not induce vomiting and seek medical advice immediately.

4.2 Most important symptoms and effects, both acute and delayed

Headache, dizziness, nausea, eye irritation

4.3 Indication of any immediate medical attention and special treatment needed

May cause irritations of the respiratory tract
Treat symptomatically and supportively

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

CO₂, dry powder, foam or water spray

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

May form toxic carbon oxides if burning.

Closed container may rupture if strongly heated.

Combustible liquid.

Vapours can travel to a source of ignition and flash back.

Explosive mixtures may occur at temperatures at or above the flashpoint.

5.3 Advice for firefighters

Cool closed containers exposed to fire with water spray.

Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment.

Avoid breathing vapours, mist or gas.

Ensure adequate ventilation

6.2 Environmental precautions

Do not allow to enter sewers, surface or ground water.

6.3 Methods and material for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste.

Keep in suitable, closed containers for disposal.

Suitable binder: sand

6.4 Reference to other sections

Section 8 for information on personal protection equipment.

Section 13 for disposal information



SECTION 7: Handling and storage

7.1 Precautions for safe handling	If possible, use material transfer, metering and blending plants that are closed. Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
7.2 Conditions for safe storage, including any incompatibilities	
Advice on protection against fire and explosion	Follow normal measures for preventive fire protection.
Storage	Store in a cool place. Keep container tightly closed in a dry and well-ventilated place. Residual vapours might explode on ignition; do not apply heat, cut, drill and grind or weld on or near this container. Mechanical exhaust required.
Advice on common storage	Observe prohibition against storing together!
German storage class	10- Combustible liquids
Storage stability	Stable under recommended storage conditions
7.3 Specific end use(s)	No further relevant information available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters	Occupational Exposure Limit	11 mg/m ³ (2 ppm)
8.2 Exposure controls		
Appropriate engineering controls	If possible, use material transfer, metering and blending plants that are closed	
Personal protective equipment		
Eye/ face protection	closed goggles, face shield	
Skin protection		
Hand protection	Type of material	Thickness
	Butyl-rubber	0.5 mm
	Polychloroprene (PCP)	0.5 mm
		Breakthrough time
		> 480 min
		110 min
Body protection	Boots, body suit	
Respiratory protection	Respiratory equipment with suitable filter or a self-contained respiratory apparatus.	
Thermal hazards	Combustible liquid, possibility of decomposition on excess heating	
Industrial hygiene	Do not inhale vapours / aerosols. Avoid contact with skin and eyes. Remove immediately all contaminated clothing. Use disposable clothing if appropriate. Smoking, eating and drinking should be prohibited in the application area.	

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties	
Appearance	Colourless to light yellow liquid
Odour	Peppermint-like
Odour threshold	0.2ppm
pH	no data available
Melting point	-8.1°C
Boiling point	215°C
Flash point	96°C (Closed cup)
Evaporation rate	0.02 (nBuAc=1)
Flammability (solid, gas)	not applicable (product is a liquid)
Flammability limits	Lower 0.8 Vol % Upper 3.8 Vol %
Vapour pressure	0.33 hPa at 20°C
Vapour density	4.77 (air =1 at boiling point of isophorone)
Relative density	0.9255 at 20°C
Solubility in water	12 g/l at 20°C
Partition coefficient	1.67 log Kow (n-octanol/water) at 20°C
Ignition temperature	470°C
Decomposition temperature	no data available

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Viscosity at 20 °C	2.83 mm ² /s
Explosive properties	no explosive properties however containers may explode in fire
Oxidizing properties	no oxidizing properties
9.2 Other information	
Heat of combustion	-16,170 BTU/lb= -8,980 cal/g= -376x10+5 J/kg
Heat of vaporization	43.4 kJ/mol

SECTION 10: Stability and reactivity

10.1 Reactivity	No hazardous reaction when handled and stored according to provisions.
10.2 Chemical stability	Under storage at normal ambient temperatures (-40°C to +40°C), the product is stable.
10.3 Possibility of hazardous reactions	No known hazardous reactions if used as directed
10.4 Conditions to avoid	Avoid excessive heat and sources of ignition
10.5 Incompatible materials	None known
10.6 Hazardous decomposition products	Thermal decomposition products- carbon oxides

SECTION 11: Toxicological information

11.1 Information on toxicological effects	
Acute toxicity	
LD50 oral rat	1500 mg/kg bw harmful
LC50 inhalation rat	7 mg/l not classified
LD50 Dermal rabbit	1200 mg/kg bw harmful
Mortality Aspiration rat	0.2ml 60%
Skin irritation	Mild skin irritation 24 h (rabbit)
Serious eye irritation	moderate eye irritation - 24 h (rabbit)
Respiratory or skin sensitization	No sensitizing effects known
Germ cell mutagenicity	non mutagenic (Ames test)
Carcinogenicity	Carc. Cat. 2, suspected of causing cancer (male rat)
Reproductive toxicity	no adverse effect on reproduction (rat)
STOT-single exposure	irritating to eye and skin; Category 3 respiratory tract irritation
STOT-repeated exposure	not classified as specific target organ toxicant
	NOAEL 102.5 mg/kg bw/day; rat (oral)
	NOAEC 28 d for rats <208 mg/m ³ (inhalation)
	NOAEL 150 mg/kg bw/day (dog)
Aspiration hazard	hazardous, 60% mortality at 0.2ml dose

SECTION 12: Ecological information

12.1 Toxicity	
Aquatic toxicity	
Toxicity to fish	LC50 96h 228mg/L <i>Pimephales promelas</i>
Toxicity to aquatic invertebrates	LC50 48h 120 mg/L <i>Daphnia magna</i>
Toxicity to aquatic algae and cyanobacteria	EC50 72h 475 mg/L <i>Desmodesmus subspicatus</i>
Toxicity to microorganisms	EC50 3h 100mg sewage, domestic
Long term toxicity to fish	NOEC 35d 11mg/L <i>Pimephales promelas</i>
12.2 Persistence and degradability	
Biodegradation	readily biodegradable (95% in 28days)
12.3 Bioaccumulative potential	Bioconcentration factor 7; Half-life <1 day; bluegill sunfish (<i>Lepomis macrochirus</i>)
	very low potential for bioaccumulation
12.4 Mobility in soil	Koc = 58.32; very low potential for geoaccumulation (Blume scale)
12.5 Results of PBT and vPvB assessment	Not a PBT, vPvB substance according to the REACH regulation
12.6 Other adverse effects	No further information available



SECTION 13: Disposal considerations

13.1 Waste treatment methods	Observe all federal, state, and local environmental regulations. 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. Do not dispose in sewage.
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◆ **SECTION 14: Transport information**

	ADR/RID	IMDG	ICAO/IATA
14.1 UN Number	-	-	-
14.2 UN proper shipping name	not hazardous for transport		
14.3 Transport hazard class	-	-	-
14.4 Packaging group	-	-	-
14.5 Environmental hazards	not environmentally hazardous, not a marine pollutant		
14.6 Special precautions for the user	Combustible liquid; Flash point 96°C (closed cup)		
14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	See regulatory information for transport approval		

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture		
Major accident hazard	Seveso III	no

International Chemical Inventory Status

USA (TSCA)	listed
Canada (DSL)	listed
Australia (AICS)	listed
Japan (MITI)	listed
Korea (KECL)	listed
Philippines (PICCS)	listed
China	listed
New Zealand	listed
Taiwan	listed

15.2 Chemical safety assessment	A Chemical Safety Assessment will be carried out at the time of REACH registration
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SECTION 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.

Further information:

Sections in which changes have been made since the last version are marked with a diamond ◆ in the left hand margin.

Abbreviations and acronyms in English language:

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
AICS	Australian Inventory of Chemical Substances
CAS	Chemical Abstracts Service (division of the American Chemical Society)
CLP	Classification for Labeling and Packaging
DSL	Domestic Substances List
EC	European Commission
EC50	Half maximal effective concentration
EINECS	European Inventory of Existing Commercial Chemical Substances
GHS	Globally Harmonized System of Classification and Labeling of Chemicals
IATA	International Air Transport Association
IBC	International Bulk Chemical
ICAO	International Civil Aviation Organization
IMDG	International Maritime Code for Dangerous Goods
KECL	Korea Existing Chemicals List
KOC	Soil adsorption coefficient
KOW	Partition Coefficient octanol-water
LC50	Lethal concentration, 50 percent

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LD50	Lethal dose, 50 percent
MARPOL	International Convention for the Prevention of Pollution from Ships
MITI	Ministry of International Trade and Industry
NOAEC	No Observed Adverse Effect Concentration
NOAEL	No Observed Adverse Effect Level
NOEC	No Observed Effect Concentration
PBT	Persistent, bioaccumulative and toxic substances
PICCS	Philippine Inventory of Chemicals and Chemical Substances
RID	Regulations Concerning the International Transport of Dangerous Goods by Rail
STOT	Specific target organ toxicity
TSCA	Toxic Substances Control Act
UN	United Nations
vPVB	(very) Persistent, (very) Bioaccumulative

Sources

Commission Regulation (EU) 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

ECHA	https://echa.europa.eu/registration-dossier/-/registered-dossier/14527
Chemid	https://chem.nlm.nih.gov/chemidplus/rn/78-59-1
HSDB	https://toxnet.nlm.nih.gov/cgi-bin/sis/search2/r?dbs+hsdb:@term+@rn+@rel+78-59-1
CDC	https://www.cdc.gov/niosh/docs/81-123/pdfs/0355.pdf
