

Safety data sheet as per Commission Regulation (EU) 2020/878

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

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

Relevant identified uses	Industrial Use: For manufacture of chemicals Professional use: Solvent in printing inks, paints, lacquers, adhesives, copolymers, coatings, finishings and pesticides; Ingredient in wood preservatives and floor sealants Chemical intermediate; coating products, inks and toners, plant protection products and washing & cleaning products
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 Limited Prasol House, Plot No.A-17/2/3, T.T.C. Indl. Area, Khairne M.I.D.C., Navi Mumbai - 400 710. Maharashtra, India.
Telephone	+91-22-27782555/ 61952500
Telefax	+91-22-61952577
e-mail address	sales@prasolchem.com; inquiry@prasolchem.com

1.4 Emergency telephone number

Telephone	+91-22- 27782555/ 61952500
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
Specific Target Organ Toxicity	Category 3	H335	May cause respiratory irritation
Carcinogenicity	Category 2	H351	Suspected of causing cancer

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
Warning



GHS08

Signal word

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

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Storage	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.
Disposal	P370+P378	In case of fire: Use CO ₂ , dry powder, foam or water spray to extinguish
	P403	Store in a well-ventilated area.
	P405	Store locked up.
	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 Annex XIII to REACH regulation

Under assessment as Endocrine Disrupting as per criteria of Delegated Regulations (EC) 2017/2100 or (EC) 2018/605

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

CAS Number	78-59-1
EC Number	201-126-0
Molecular Formula	C ₉ H ₁₄ O
Molecular Weight	138.21

Ingredient	Classification	Concentration (%)	SCL, M-factor, ATE
3,5,5-trimethylcyclohex-2-enone (isophorone)	Acute Tox. Oral 4, Acute Tox Der. 4, Eye Irrit. 2, Carc. 2, STOT SE 3 H302, H312, H319, H335, H351	98.5 min	STOT SE 3; H335: C ≥ 10 %
3,5,5-trimethylcyclohex-3-en-1-one (β-isophorone)	Acute Tox.Oral 4, Acute Tox. Der. 4, Acute Tox. Inh. 3, Eye Irrit. 2A, STOT SE 3, Carc. 2 H302, H312, H319, H331, H335, H351	1.5 max	

There are no other ingredients present, which are classified as hazardous and hence require reporting in this section.

3.2 Mixtures

not applicable
None of the ingredients present are classified as skin sensitisers 1A, respiratory sensitisers 1A and aspiration hazards. The substance is under assessment as endocrine disrupter.

SECTION 4: FIRST AID MEASURES

4.1 Description of first aid measures

General information

Take off all contaminated clothing immediately.
After inhalation 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

May cause irritations of the respiratory tract

After inhalation May cause respiratory irritation.

After skin contact Repeated exposure to this material can result in absorption through skin causing significant health hazard. Skin contact may aggravate preexisting dermatitis.

Red skin. Tingling/irritation of the skin.

After eye contact Irritation of the eye tissue. Inflammation/damage of the eye tissue.

After swallowing AFTER INGESTION OF HIGH QUANTITIES: Vomiting. Nausea. Disturbances of consciousness

Chronic symptoms Skin rash/inflammation

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically and supportively

SECTION 5: FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media CO₂, dry powder, foam or water spray

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- 5.2 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** For small spills and large spills: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Clear spills immediately
Avoid breathing vapours, mist or gas.
Ensure adequate ventilation
- For non-emergency personnel** Protective equipment: Gloves, Face shield, Protective clothing.
Emergency procedures: Mark the danger area. No naked flames. Wash contaminated clothes.
- For emergency responders** Protective equipment: Equip cleanup crew with proper protection.
Emergency procedures: Ventilate area.
- 6.2 Environmental precautions** Do not allow to enter sewers, surface or ground water.
- 6.3 Methods and material for containment and cleaning up** For containment: Contain released product, collect/pump into suitable containers.
Plug the leak, cut off the supply.
For cleaning up: Soak up with inert absorbent material eg. sand, earth, vermiculite or powdered lime stone and keep in suitable, closed containers for disposal. Clean contaminated surfaces with an excess of water. Wash clothing and equipment after handling.
- 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.
- Protective measures** Measures to prevent fire: Keep away from naked flames/heat. Use spark-/explosion proof appliances.
Measures to prevent aerosol and dust generation: Measure the concentration in the air regularly. Carry operations in the open/under local exhaust/ventilation or with respiratory protection. Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Thoroughly clean/dry the installation before use.
Measures to protect the environment: Keep container tightly closed. If possible, use material transfer, metering and blending plants that are closed.
- Advice on general occupational hygiene** Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
- 7.2 Conditions for safe storage, including any incompatibilities**
- Technical measures and storage conditions** Keep only in the original container in a cool, well ventilated place away from ignition sources and incompatible materials. Keep container closed when not in use.
Follow normal measures for preventive fire protection.
- Packaging material** SUITABLE MATERIAL: steel, stainless steel, carbon steel, aluminium, glass
- Incompatible products** Copper may be attacked. Attacks plastics
- Advice on common storage** Observe prohibition against storing together!
- Storage stability** Stable under recommended storage conditions
- Storage class** 10 Combustible liquid
- 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/m³ (2 ppm)
- DNEL/DMEL (Workers)**
- Acute - local effects, inhalation 22 mg/m³



Long-term - systemic effects, dermal	13 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	11 mg/m ³
Long-term - local effects, inhalation	11mg/m ³
DNEL/DMEL (General population)	
Acute - local effects, inhalation	0.7 mg/m ³
Long-term - systemic effects, oral	0.325 mg/kg bodyweight/day
Long-term - systemic effects, inhalation	0.7 mg/m ³
Long-term - systemic effects, dermal	No hazard identified
Long-term - local effects, inhalation	0.7 mg/m ³
PNEC (Water)	
PNEC aqua (freshwater)	0.089 mg/l
PNEC aqua (marine water)	0.009 mg/l
PNEC (Sediment)	
PNEC sediment (freshwater)	0.839 mg/kg dwt
PNEC sediment (marine water)	0.084 mg/kg dwt
PNEC (Soil)	
PNEC soil	0.12 mg/kg dwt
PNEC (STP)	
PNEC sewage treatment plant	1 mg/l

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	Breakthrough time
	Butyl-rubber	0.5 mm	> 480 min
	Polychloroprene (PCP)	0.5 mm	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

Physical state	Liquid
Color	Colourless to light yellow
Odour	Peppermint-like
Odour threshold	0.2ppm
Melting point	-8.1°C
Boiling point	215°C
Flammability (solid, gas)	not applicable (product is a liquid)
Lower and upper explosion limit	0.8 - 3.8 v/v%
Flash point	96°C (Closed cup)
Ignition temperature	470°C
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity at 20°C	2.83 mm ² /s
Solubility in water	12 g/l at 20°C
Partition coefficient	1.67 log Kow (n-octanol/water) at 20°C
Vapour pressure	0.33 hPa at 20°C
Relative density	0.9255 at 20°C
Relative vapour density	4.77 (air =1 at boiling point of isophorone)
Particle characteristics	Not applicable (substance is a liquid)

9.2 Other information

Evaporation rate	0.02 (nBuAc=1)
Explosive properties	no explosive properties based on chemical structure

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Oxidizing properties	no oxidizing properties based on chemical structure
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 hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

LD50	oral	rat	1500 mg/kg bw	Category 4, H302
LC50	inhalation	rat	7 mg/l	not classified
LD50	Dermal	rabbit	1200 mg/kg bw	Category 4, H312
Mortality	Aspiration	rat	0.2ml	60%

Skin irritation

Mild skin irritation 24 h (rabbit)

Serious eye irritation

serious eye irritation - 24 h (rabbit) **Category 2, H319**

Respiratory or skin sensitization

No sensitizing effects known

Germ cell mutagenicity

non mutagenic (Ames test)

Carcinogenicity

Suspected of causing cancer (in male rat by a mechanism not relevant to humans) **Category 2, H351**

Reproductive toxicity

no adverse effect on reproduction (rat)

STOT-single exposure

Category 3 respiratory tract irritation conc. >10%, H335

STOT-repeated exposure

not classified as specific target organ toxicant for repeated exposure

NOAEL 102.5 mg/kg bw/day; rat (oral)

NOAEC 28 d for rats <208 mg/m³ (inhalation)

NOAEL 150 mg/kg bw/day (dog)

Aspiration hazard

hazardous, 60% mortality at 0.2ml dose

11.2 Information on other hazards

Endocrine disrupting properties

Under assessment as Endocrine Disrupting

Other information

No further information

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 after 14 days of exposure 7; Half-life <1 day; bluegill 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 Endocrine disrupting properties

Under assessment as Endocrine Disrupting

12.6 Other adverse effects

No further information available

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SECTION 13: DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods	Observe all federal, state, and local environmental regulations.
Product disposal	Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
Packaging disposal	Clean container with water. Recover waste water for processing later. Destroy packaging by incineration at an approved waste disposal site.
Sewage disposal	Do not dispose in sewage.

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 Maritime transport in bulk according to IMO instruments	Ship type: 3; Pollution Category: Y		

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 (Tracking No 7187)
Canada (DSL)	listed
Australia (AICS)	listed
Japan (MITI)	Listed (MITI No. 3-2381)
Korea (KECL)	Listed (KE No. KE-34467)
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

SECTION 16: OTHER INFORMATION

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

Abbreviations and acronyms:

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
AICS	Australian Inventory of Chemical Substances
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (division of the American Chemical Society)
CLP	Classification for Labeling and Packaging
DMEL	Derived minimal effect level
DNEL	Derived No-Effect Level
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

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LC50	Lethal concentration, 50 percent
LD50	Lethal dose, 50 percent
M-factor	Multiplication Factor
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
PNEC	Predicted No-Effect Concentration
RID	Regulations Concerning the International Transport of Dangerous Goods by Rail
SCL	Specific concentration limit
STOT	Specific target organ toxicity
TSCA	Toxic Substances Control Act
UN	United Nations
vPVB	(very) Persistent, (very) Bioaccumulative

Key literature references and sources for data

Commission Regulation (EU) 2020/878 of 18 June 2020 amending Annex II to Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning 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>

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