

**Safety data sheet as per COMMISSION REGULATION (EU) No 453/2010
of 20 May 2010 amending Regulation (EC) No 1907/2006**

Product: Isophorone



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

1.1 Product details

Trade name: Isophorone/ 3,5,5-trimethylcyclohex-2-enone

CAS No.: 78-59-1

EC No.: 201-126-0

Pre-Registration number 05-2114672544-43-0000

1.2 Relevant identified uses of the substance or mixture and uses advised against Agriculture, forestry and fishing (SU 1); Manufacture of bulk, large scale chemicals (including petroleum products) (SU 8); Manufacture of fine chemicals(SU 9)

Uses identified against: Cosmetic use

1.3 Details of the supplier of the safety data sheet:

Manufacturer/Supplier:

Prasol Chemicals Ltd.,
Prasol House, Plot No.A-17/2/3,
T.T.C. Indl. Area, Khairne M.I.D.C.,
Navi Mumbai - 400 710,
Maharashtra, India.
Tel: +91-22-27782555
Fax: +91-22-27782430

Further information obtainable from:

Mr. Dhaval Parikh

e-mail:sales@prasolchem.com; inquiry@prasolchem.com

Information in case of emergency:

Product safety department Tel: +91-22- 27782555; Fax: +91-22- 27782430

Other Comments (e.g. language(s) of the phone service): English

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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



GHS07

Acute Tox. 4

Acute Tox. 4

Eye Irrit. 2

Carc. 2

STOT SE 3



GHS08

H302 Harmful if swallowed

H312 Harmful in contact with skin.

H319 Causes serious eye irritation.

H351 Suspected of causing cancer

H335 May cause respiratory irritation

2.1.2 Classification according to Directive 67/548/EEC or Directive 1999/45/EC



Xn; Harmful



Xi; Irritant

Carc. Cat. 3

R21/22 Harmful in contact with skin and if swallowed.

R36/37 Irritating to eyes and respiratory system

R40 Limited evidence of a carcinogenic effect.

Information concerning particular hazards for human and environment: Not applicable

2.2 Label elements

Labeling according to Regulation (EC) No 1272/2008

Hazard pictograms



GHS07



GHS08

Signal word Warning

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Hazard-determining components of labeling: Void

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

P261 Avoid breathing dust/fume/gas/mist/vapors/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P281 Use personal protective equipment as required.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P405 Store locked up

P501 Dispose of contents/container in accordance with local/regional/national/international regulations

Labeling according to EU guidelines:

The product has been classified and marked in accordance with EU Directives / Ordinance on Hazardous Materials.

Code letter and hazard designation of product:



Carc. Cat. 3

Xn Harmful

Risk phrases:

21/22 Harmful in contact with skin and if swallowed.

36/3 7 Irritating to eyes and respiratory system.

40 Limited evidence of a carcinogenic effect.

2.3 Other hazards

Results of PBT and vPvB assessment: Not applicable

SECTION 3: Composition/information on ingredients

Chemical characterization:

CAS No. Description
78-59-1 3,5,5-trimethylcyclohex-2-enone

Identification number(s)

EC Number: 201-126-0

Index number: 606-012-00-8

Additional information:

Molecular Formula: C₉H₁₄O

Molecular Weight: 138.21

SECTION 4: First aid measures

4.1 General information: Consult a physician. Show this safety data sheet to the doctor in attendance.

After inhalation:

If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.

After skin contact:

In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

After eye contact:

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.

After swallowing:

INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-

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mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive.

Information for doctor: Treat symptomatically and supportively.

4.2 Most important symptoms and effects, both acute and delayed

Burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis.

4.3 Indication of any immediate medical attention and special treatment needed No further relevant information available

SECTION 5: Firefighting measures

5.1 Suitable extinguishing agents:

CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

For safety reasons unsuitable extinguishing agents: Water jet.

5.2 Special hazards arising from the substance or mixture May form Carbon oxides

5.3 Protective equipment: 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 vapors, 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.

6.4 Reference to other sections:

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information

SECTION 7: Handling and storage

7.1 Precautions for safe handling:

Avoid contact with skin and eyes.

Avoid inhalation of vapor or mist.

Information about fire - and explosion protection: Normal measures for preventive fire protection.

7.2 Conditions for safe storage, including any incompatibilities:

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Information about storage in one common storage facility:

Always store away from incompatible compounds such as oxidizing agents, acids, alkalis (bases).

Further information about storage conditions: Mechanical exhaust required.

7.3 Specific end use(s) No further relevant information available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Additional information about design of technical facilities:

Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash station and safety shower is proximal to the work- station location.

Ingredients with limit values that require monitoring at the workplace: Not required.

Additional information: The lists valid during the making were used as basis.

8.2 Exposure controls

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.

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Avoid contact with the eyes and skin.

Respiratory protection:

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Protection of hands: Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Material of gloves

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

Eye protection: Tightly sealed goggles

Body protection: Choose body protection according to the amount and concentration of the dangerous substance at the work place.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

General Information

Appearance	: Colorless to light yellow liquid
Odour	: Peppermint-like
Odour threshold	: 0.2ppm
pH	: no data available
Melting point/Melting range	: -8.1°C
Boiling point/Boiling range	: 215°C
Flash point	: 96°C (Closed cup)
Evaporation rate	: 0.02 (nBuAc=1)
Flammability (solid, gas)	: not applicable
Upper/lower flammability or explosive limits:	
Lower: 0.8 Vol %	
Upper: 3.8 Vol %	
Vapour pressure at 20°C	: 0.33 hPa
Vapour density	: 4.77 (air =1 at boiling point of isophorone)
Relative density at 20°C	: 0.9255
Solubility in / Miscibility with water at 20°C:	12 g/l
Partition coefficient (n-octanol/water) at 23°C:	2.86 log POW
Ignition temperature	: 470°C
Decomposition temperature	: no data available
Viscosity at 20 °C	: 2.83 mm ² /s
Explosive properties	: Containers may explode in fire
Oxidising properties	: no data available

9.2 Other information No further relevant information available

SECTION 10: Stability and reactivity

10.1 Reactivity

No dangerous reactions known.

10.2 Chemical stability

Under storage at normal ambient temperatures (minus 40° C to + 40° C), the product is stable.

No hazardous reaction when handled and stored according to provisions.

10.3 Possibility of hazardous reactions

No known hazardous reactions

10.4 Conditions to avoid:

Avoid excessive heating.

10.5 Incompatible materials:

Strong oxidizing agents, strong acids, strong alkalis (bases).

10.6 Hazardous decomposition products:

Carbon oxides

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity:

LD50	Oral	rat	2330 mg/kg
LD50	Dermal	rabbit	1500 mg/kg
LC50	Inhalative	rat	7000mg/m3

Skin corrosion/irritation: Mild skin irritation 24 h (rabbit)

Serious eye damage/irritation: Eye irritation - 24 h (rabbit)

Respiratory or skin sensitization: No sensitizing effects known

Acute effects (acute toxicity, irritation and corrosivity)

Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction) Carc. Cat. 3

Additional information: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated

SECTION 12: Ecological information

12.1 Toxicity

Aquatic toxicity

LC50	48hr	120 mg/l (Daphnia Magna)
LC50	96 h	228mg/l (Fathead Minnow)

12.2 Persistence and degradability

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: 1.70 (exp database) Log Kaw used: -3.566 (exp database)

Log Koa (KOAWIN v1.10 estimate): 5.266

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10): Biowin1 (Linear Model):0.5046

Biowin2 (Non-Linear Model) : 0.2441

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.6591 (weeks-months) Biowin4 (Primary Survey Model) : 3.4727 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) :

Behavior in environmental systems:

12.3 Bio accumulative potential:

very low potential for bioaccumulation; bluegill sunfish (*Lepomis macrochirus*)

12.4 Mobility in soil

Soil Adsorption Coefficient (PCKOCWIN v1.66): Koc: 58.32

Log Koc: 1.766

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure

Bioaccumulation Estimates from Log Kow (BCFWIN v2.17):

Log BCF from regression-based method = 0.609 (BCF = 4.064)

log Kow used: 1.70 (expkow database)

Volatilization from Water:

Henry LC: 6.64E-006 atm-m3/mole (Henry experimental database)

Half-Life from Model River: 104.9 hours (4.369 days)

Half-Life from Model Lake : 1243 hours (51.77 days)

Removal In Wastewater Treatment:

Total removal: 2.41 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.95 percent

Total to Air: 0.37 percent (using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount	Half-Life	Emissions
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	(percent)	(hr)	(kg/hr)
Air	0.14	1.72	1000
Water	37.6	900	1000
Soil	62.1	1.8e+003	1000
Sediment	0.109	8.1e+003	0

Persistence Time: 674 hr

Additional ecological information: readily biodegradable (95% degradation within 28 days)

General notes:

Water hazard class 2 (German Regulation) (Assessment by list): hazardous for water

12.5 Results of PBT and vPvB assessment To be provided after the REACH registration

12.6 Other adverse effects No further relevant information available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product:

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.

Contaminated packaging: Disposal must be made according to official regulations.

SECTION 14: Transport information

Land Transport (ADR/RID)

Marine Transport (IMDG)

Air Transport (ICAO/ IATA)

14.1 UN/ID Number: -

14.2 UN proper shipping name: Not dangerous goods in transport regulations

14.3 Transport hazard class: -

14.4 Packaging group: -

14.5 Environmental hazards: none; not a marine pollutant

14.6 Special precautions for the user: no data available

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code: not applicable

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006

Hazard pictograms Please refer section 2

Signal word Warning

Hazard statements Please refer section 2.

Labeling according to EU guidelines:

Code letter and hazard designation of product: Xn; Harmful

Risk phrases: Please refer section 2

15.2 Chemical safety assessment A Chemical Safety Assessment has not been carried out.

National regulations:

Other regulations, limitations and prohibitive regulations

Substances of very high concern (SVHC) according to REACH, Article 57: The substance is not listed as SVHC.

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.

Department issuing MSDS:

Product safety department.

Contact:

Tel: +91-022-27782555

Fax: +91-022-27782430

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Abbreviations and acronyms:

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

GHS: Globally Harmonized System of Classification and Labeling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

Sources

REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL on classification, labeling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006

Sigma MSDS :

<http://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=IN&language=en&productNumber=118709&brand=ALDRICH&PageToGoToURL=http%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Faldrich%2Fi18709%3Flang%3Den>

Dow data sheet: http://msdssearch.dow.com/PublishedLiteratureDOWCOM/dh_0119/0901b803801195d7.pdf?filepath=oxy-solvents/pdfs/noreg/327-00030.pdf&fromPage=GetDoc

Acros MSDS

http://www.acros.com/DesktopModules/Acros_Search_Results/Acros_Search_Results.aspx?search_type=ProductNumber&SearchString=12264

TCI MSDS <http://www.tci-america.com/msds/search>

Chemid <http://chem.sis.nlm.nih.gov/chemidplus/rn/78-59-1>

Chemcas <http://www.chemcas.org/drug/analytical/cas/78-59-1.asp>

Cdc <http://www.cdc.gov/niosh/docs/81-123/pdfs/0355.pdf>

Toxnet <http://toxnet.nlm.nih.gov/cgi-bin/sis/search2/r?dbs+hsdb:@term+@rn+@rel+78-59-1>

Goodscents <http://www.thegoodscentscompany.com/data/rw1036811.html>

Lookchem <http://www.lookchem.com/ISOPHORONE/Uses>

Data compared to the previous version altered.

- Section 1: Identification of the substance/mixture and of the company/undertaking
- Section 2: Hazard Identification
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