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

Product details
Trade name: 3,5,5-trimethylcyclohex-2-enone
CAS No.: 78-59-1
EC No.: 201-126-0
Pre-Registration number 05-2114672544-43-0000

Application of the substance / the preparation
- It is used as a solvent in some printing inks, paints, lacquers, adhesives, copolymers, coatings, finishings and pesticides.
- It is also used as a chemical intermediate and as an ingredient in wood preservatives and floor sealants.

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:
Contact details of European importer:
Emergency telephone number:
Telephone number of EU importer:
Opening hours:
Other Comments (e.g. language(s) of the phone service): English

2 Hazards identification

Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008

GHS08 health hazard
Carc. 2 H351 Suspected of causing cancer

GHS07
Acute Tox. 4 H302 Harmful if swallowed
Acute Tox. 4 H312 Harmful in contact with skin.
Eye Irrit. 2 H319 Causes serious eye irritation.
STOT SE 3 H335 May cause respiratory irritation

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

Xn: Harmful
R21/22-40: Harmful in contact with skin and if swallowed. Limited evidence of a carcinogenic effect.

Xi: Irritant
R36/37: Irritating to eyes and respiratory system

Carc. Cat. 3

Information concerning particular hazards for human and environment: Not applicable

Label elements

Revision: 14-01
Issue Date: 05.05.2014
Hazard pictograms

GHS07  GHS08

Signal word Warning

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.
36/37 Irritating to eyes and respiratory system.
40 Limited evidence of a carcinogenic effect.

Safety phrases:
2 Keep out of the reach of children
13 Keep away from food, drink and animal feeding stuffs.
23 Do not breathe gas/fumes/vapors/spray (appropriate wording to be specified by the manufacturer).
36/37/39 Wear suitable protective clothing, gloves and eye/face protection

3 Chemical characterization:

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

Identification number(s)
EINECS Number: 201-126-0
Index number: 606-012-00-8

Additional information:
Molecular Formula: C9H14O
Molecular Weight: 138.21

4 First aid measures

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-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.
The following symptoms may occur:
Burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis.

5 Firefighting measures

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.

Protective equipment: Wear self-contained breathing apparatus.

6 Accidental release measures

Person-related safety precautions:
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

Measures for environmental protection: Do not allow to enter sewers/surface or ground water.

Measures for cleaning/collecting:
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

7 Handling and storage

Handling:
Information 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.

Storage:
Requirements to be met by storerooms and receptacles:
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.

Specific applications:
-It is used as a solvent in some printing inks, paints, lacquers, adhesives, copolymers, coatings, finishings and pesticides.
-It is also used as a chemical intermediate and as an ingredient in wood preservatives and floor sealants.

8 Exposure controls/personal protection

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.

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.
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.

9 Physical and chemical properties

General Information
Appearance:
Form: Liquid
Color: Colorless to white
Odor: Peppermint-like

Change in condition
Melting point/Melting range: -8.1°C
Boiling point/Boiling range: 215°C
Flash point: 96°C (Closed cup)
Ignition temperature: 460°C
Danger of explosion: Containers may explode in fire

Explosion limits:
Lower: 0.8 Vol %
Upper: 3.8 Vol %

Vapor pressure at 20°C: 0.33 hPa
Density at 20°C: 0.92 g/cm³
Solubility in / Miscibility with water at 20°C: 12 g/l

10 Stability and reactivity

Thermal decomposition / conditions to be avoided: Avoid excessive heating.

Materials to be avoided:
Strong oxidizing agents, strong acids, strong alkalis (bases).

Dangerous reactions No dangerous reactions known.

Dangerous decomposition products: Carbon oxides.
11 Toxicological information

Acute toxicity:

<table>
<thead>
<tr>
<th>LD/LC50 values relevant for classification:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral</td>
</tr>
<tr>
<td>Dermal</td>
</tr>
<tr>
<td>Inhalative</td>
</tr>
</tbody>
</table>

Primary irritant effect:
- **on the skin**: Skin - rabbit - Mild skin irritation - 24 h
- **on the eye**: Eyes - rabbit - Eye irritation - 24 h

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

12 Ecological information

Information about elimination (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:

Behavior in environmental systems:
Mobility and bioaccumulation potential:
Soil Adsorption Coefficient (PCKOCWIN v1.66):
- Log Koc: 1.266
- Koc = 58.82
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)

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:

<table>
<thead>
<tr>
<th>Mass Amount (percent)</th>
<th>Half-Life (hr)</th>
<th>Emissions (kg/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.14</td>
<td>1.72</td>
</tr>
<tr>
<td>Water</td>
<td>37.6</td>
<td>900</td>
</tr>
<tr>
<td>Soil</td>
<td>62.1</td>
<td>1.8e+003</td>
</tr>
<tr>
<td>Sediment</td>
<td>0.109</td>
<td>8.1e+003</td>
</tr>
</tbody>
</table>
PRASOL CHEMICALS LIMITED
Material Safety Data Sheet
Product: Isophorone

Persistence Time: 674 hr

Ecotoxical effects:

<table>
<thead>
<tr>
<th>Aquatic toxicity classification:</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC50 (96hr)</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

Additional ecological information:

General notes:
Water hazard class 2 (German Regulation) (Assessment by list): hazardous for water
Do not allow product to reach ground water, water course or sewage system. Danger to drinking water if even small quantities leak into the ground

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

13 Disposal considerations

Product:
Recommendation
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.

Uncleaned packaging:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

Land transport ADR/RID (cross-border)
ADR/RID class:-

Maritime transport IMDG:
IMDG Class:-
Marine pollutant: No

Air transport ICAO-TI and IATA-DGR:
ICAO/IATA Class:
UN "Model Regulation":

15 Regulatory information

Labeling according to Regulation (EC) No 1272/2008
Hazard pictograms Please refer section 2
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.

Labeling according to EU guidelines:
Code letter and hazard designation of product: Xn; Harmful

Risk phrases:
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.

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.
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

**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
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**

Sigma MSDS http://www.sigmaaldrich.com/catalog/DisplayMSDSContent.do
TCI MSDS http://www.tciamerica.com/msds/search
Chemid http://chem.sis.nlm.nih.gov/chemidplus/ProxyServlet?objectHandle=Search&actionHandle=getAll3DMViewFiles&nextPage=jsp%2F%2Fcommon%2FChemFull.jsp%3FcalledFrom%3D3D&ite&chemid=0000078591&formatType=3D
Chemspider http://www.chemspider.com/RecordView.aspx?rid=6d9b3f62-3f5f-4f36-a0e7-6234bc99a81a
Chemcas http://www.chemcas.org/dump/analytical/cas/78-59-1.asp
Toxnet http://toxnet.nlm.nih.gov/cgi-bin/sis/searchf?/temp/~V74kBX: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
- Section 3: Composition/Information on ingredients
- Section 4: First-aid measures.
- Section 5: Fire-fighting measures
- Section 6: Accidental Release measures
- Section 7: Handling and storage.
- Section 8: Exposure Controls/Personal protection.
- Section 9: Physical and Chemical properties.
- Section 10: Stability and Reactivity.
- Section 11: Toxicological Information.
- Section 12: Ecological Information.
- Section 13: Disposal consideration
- Section 14: Transport information
- Section 15: Regulatory information