1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

- **Product name**: Isophorone
- **Product Number**: I18709
- **Brand**: Aldrich
- **Index-No.**: 606-012-00-8
- **CAS-No.**: 78-59-1

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

- **Identified uses**: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

- **Company**: Sigma-Aldrich
  3050 Spruce Street
  SAINT LOUIS MO 63103
  USA
- **Telephone**: +1 800-325-5832
- **Fax**: +1 800-325-5052

1.4 Emergency telephone number

- **Emergency Phone #**: (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

- **GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**
  - Acute toxicity, Oral (Category 4), H302
  - Acute toxicity, Dermal (Category 4), H312
  - Eye irritation (Category 2A), H319
  - Carcinogenicity (Category 2), H351
  - Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

- **Pictogram**: 
  - Signal word: Warning

- **Hazard statement(s)**
  - H302 + H312: Harmful if swallowed or in contact with skin
  - H319: Causes serious eye irritation.
  - H335: May cause respiratory irritation.
  - H351: Suspected of causing cancer.

- **Precautionary statement(s)**
  - P201: Obtain special instructions before use.
  - P202: Do not handle until all safety precautions have been read and understood.
Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
Wash skin thoroughly after handling.
Do not eat, drink or smoke when using this product.
Use only outdoors or in a well-ventilated area.
Wear protective gloves/ protective clothing/ eye protection/ face protection.
IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
Rinse mouth.
IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
IF exposed or concerned: Get medical advice/ attention.
Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Get medical advice/ attention.
Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Get medical advice/ attention.
Wash contaminated clothing before reuse.
Store in a well-ventilated place. Keep container tightly closed.
Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Synonyms : 3,5,5-Trimethyl-2-cyclohexen-1-one
Formula : C₉H₁₄O
Molecular weight : 138.21 g/mol
CAS-No. : 78-59-1
EC-No. : 201-126-0
Index-No. : 606-012-00-8

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isophorone</td>
<td>Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H302 + H312, H319, H335, H351</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

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. Evacuate personnel to safe areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials 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
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): Combustible liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isophorone</td>
<td>78-59-1</td>
<td>C</td>
<td>5.000000 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks
Central Nervous System impairment
Upper Respiratory Tract irritation
Eye irritation
Malaise
Fatigue
Confirmed animal carcinogen with unknown relevance to humans
<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>USA. NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TWA</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td>PEL</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

The value in mg/m3 is approximate.

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

   Full contact
   Material: butyl-rubber
   Minimum layer thickness: 0.3 mm
   Break through time: 480 min
   Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

   Splash contact
   Material: Nature latex/chloroprene
   Minimum layer thickness: 0.6 mm
   Break through time: 50 min
   Material tested:Lapren® (KCL 706 / Aldrich Z677558, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose 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 face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

   a) Appearance
   Form: liquid, clear
   Colour: light yellow
b) Odour No data available
c) Odour Threshold No data available
d) pH No data available
e) Melting point/freezing point Melting point/range: -8 °C (18 °F) - lit.
f) Initial boiling point and boiling range 213 - 214 °C (415 - 417 °F) - lit.
g) Flash point 96.0 °C (204.8 °F) - closed cup
h) Evaporation rate No data available
i) Flammability (solid, gas) No data available
j) Upper/lower flammability or explosive limits Upper explosion limit: 3.8 % (V)
Lower explosion limit: 0.8 % (V)
k) Vapour pressure 1.3 hPa (1.0 mmHg) at 38.0 °C (100.4 °F)
0.3 hPa (0.2 mmHg) at 20.0 °C (68.0 °F)
l) Vapour density No data available
m) Relative density 0.923 g/cm3 at 25 °C (77 °F)
n) Water solubility No data available
o) Partition coefficient: n-octanol/water No data available
p) Auto-ignition temperature 462.0 °C (863.6 °F)
q) Decomposition temperature No data available
r) Viscosity No data available
s) Explosive properties No data available
t) Oxidizing properties No data available

9.2 Other safety information
No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Strong oxidizing agents, Strong acids, Strong bases

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - No data available
In the event of fire: see section 5
11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 1,870 mg/kg
LC50 Inhalation - Guinea pig - 8 h - 4600 ppm
LD50 Dermal - Rabbit - 1,382 mg/kg
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Mild skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation - 24 h

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.
Limited evidence of carcinogenicity in animal studies

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: GW7700000
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis
Central nervous system -

12. ECOLOGICAL INFORMATION

12.1 Toxicity
Toxicity to fish
NOEC - Cyprinodon variegatus (sheepshead minnow) - 170 mg/l - 96 h
LC50 - Pimephales promelas (fathead minnow) - 145 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates
LC50 - Daphnia magna (Water flea) - 120 mg/l - 48 h

12.2 Persistence and degradability

12.3 Bioaccumulative potential
Bioaccumulation Lepomis macrochirus (Bluegill) - 14 d
- 0.0924 mg/l

Bioconcentration factor (BCF): 7

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Isophorone)
Reportable Quantity (RQ): 5000 lbs

Poison Inhalation Hazard: No

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
Isophorone CAS-No. 78-59-1 Revision Date 1993-04-24

Pennsylvania Right To Know Components
New Jersey Right To Know Components

Isophorone  CAS-No.  78-59-1  Revision Date  1993-04-24

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

| Acute Tox. | Acute toxicity |
| Carc.     | Carcinogenicity |
| Eye Irrit. | Eye irritation |
| H302      | Harmful if swallowed. |
| H302 + H312 | Harmful if swallowed or in contact with skin |
| H312      | Harmful in contact with skin. |
| H319      | Causes serious eye irritation. |
| H335      | May cause respiratory irritation. |

HMIS Rating
Health hazard:  2
Chronic Health Hazard:  *
Flammability:  1
Physical Hazard  0

NFPA Rating
Health hazard:  2
Fire Hazard:  1
Reactivity Hazard:  0

Further information
Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
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 Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.5  Revision Date: 06/02/2016  Print Date: 07/28/2016