GPS Safety Summary
Isophorone diisocyanate

Chemical Identity

Name: Isophorone diisocyanate
CAS number: 4098-71-9
Molecular formula: C\textsubscript{12}H\textsubscript{18}N\textsubscript{2}O\textsubscript{2}

Structure

![Structure of Isophorone diisocyanate]

| IUPAC name: 5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane |
| BASF brand names: Basonat I |

Product Uses

Isophorone diisocyanate is used as a raw material in the manufacture of other chemicals, particularly coating and adhesive polymers, or polyurethane foams.

Benefits

Isophorone diisocyanate can form a wide range of different types of oligomers and polymers, which can be adapted to the needs and requirements of the desired application in the coatings, leather, textile and adhesives.
Health Information

Human Health Safety Assessment

Note: The information contained in the table below may be useful to someone handling the concentrated substance such as a manufacturer or transporter. Consumers are not likely to come in contact with the concentrated substance. The data, while verifiable, are not intended to be comprehensive nor replace the data found in the (M)SDS.

<table>
<thead>
<tr>
<th>Effect Assessment</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Toxicity</td>
<td>Of low toxicity after single ingestion. Virtually nontoxic after a single skin contact. Of very high toxicity after short-term inhalation. The substance was tested in form of respirable aerosols.</td>
</tr>
<tr>
<td>Irritation</td>
<td>Causes severe skin burns and eye damage. Causes temporary irritation of the respiratory tract.</td>
</tr>
<tr>
<td>Sensitization</td>
<td>The substance may cause sensitization of the respiratory tract. Sensitization after skin contact possible.</td>
</tr>
<tr>
<td>Mutagenicity</td>
<td>The substance was mutagenic in a mammalian cell culture test system. The substance was not mutagenic in bacteria and in a test with mammals.</td>
</tr>
<tr>
<td>Toxicity after repeated exposure</td>
<td>After repeated inhalation exposure the prominent effect is local irritation of the respiratory tract.</td>
</tr>
<tr>
<td>Toxicity for reproduction</td>
<td>Repeated inhalative uptake of the substance did not cause damage to the reproductive organs. Animal studies gave no indication of a developmental toxic effect at doses that were not toxic to the parental animals.</td>
</tr>
</tbody>
</table>

Environmental Information

Environment Safety Assessment

Note: The information in this chapter is intended to provide brief and general information of this substance’s environmental impact. The results in the table below refer to testing performed with the concentrated substance. The data contained in this section explain the relative effect of the concentrated substance on the environment, as defined by certain tests.
Effect Assessment | Result  
---|---  
**Aquatic Toxicity** | Toxic to aquatic life.  
**Persistence and degradability** | Poorly biodegradable. In contact with water the substance will hydrolyse rapidly.  
**Bioaccumulation potential** | Not bioaccumulative. The statement relates to the hydrolysis products.  

**Physical/Chemical Properties**

**Phys/Chem Safety Assessment**

➢ Isophorone diisocyanate is an organic chemical substance. At ambient temperatures (including 20°C and 1013 hPa) the technical product is a liquid with a light yellowish color and a pungent smell. Isophorone diisocyanate does not have flammable or explosive properties.

*Note: The results in the table below refer to testing performed with the concentrated substance. It is not intended to be comprehensive or to replace information found in the (M)SDS.*

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>Liquid</td>
</tr>
<tr>
<td>Melting / freezing point</td>
<td>- 60 °C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>310 °C, decomposition before boiling at 260 °C</td>
</tr>
<tr>
<td>Flash point</td>
<td>150.5 °C (closed cup)</td>
</tr>
<tr>
<td>Flammability</td>
<td>Non flammable</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Non explosive</td>
</tr>
<tr>
<td>Self-ignition temperature</td>
<td>430 °C</td>
</tr>
</tbody>
</table>

**Exposure Potential**

➢ *Workplace exposure*: In general, oral, dermal as well as inhalation exposure to isophorone diisocyanate might occur. Oral exposure is unlikely to occur because it is prohibited to eat, drink or smoke in the production area. Resting rooms are separated from the manufacturing area and industrial hygiene standards are applied. As the
synthesis of isophorone diisocyanate takes place in closed continuous or closed batch processes dermal and inhalation exposure may solely arise at sampling and filling steps. Such exposure is reduced through appropriate risk management measurements like the presence of local exhaust ventilation as well as personal protection equipment (e.g. gloves and filter masks). Each manufacturing facility should have a thorough training program for employees and appropriate work processes, as well as safety equipment in place to limit unnecessary exposure. Safety showers and eye-wash stations should be accessible nearby. Workers should follow the recommended safety measures in the extended Safety Data Sheet (eSDS).

➢ **Consumer exposure:** There is no intended use of isophorone diisocyanate in consumer products. Therefore, a health hazard due to exposure for the consumer is negligible.

➢ **Environmental exposure:** Despite its poor biodegradability isophorone diisocyanate will not exist in the aquatic environment for extended time periods due to its rapid reaction in contact with water. The hydrolysis products of isophorone diisocyanate will not accumulate in the food chain. Isophorone disiocyanate is classified as acutely and chronically toxic to aquatic life. However, in a qualitative exposure assessment covering all identified uses it was demonstrated that releases into the environment do not pose a risk to aquatic life. Conclusively, all identified uses are safe for the environment based on the scientific facts summarized above and when carried out in compliance with recommended risk management measures and applicable regulations.

**Recommended Handling Measures**

*The recommended safety measures generally apply in contact with the concentrated substance. It is NOT intended to replace the comprehensive guidance found in the (M)SDS, only supplement it. Please refer to the (M)SDS for specific safety and first aid measures.*

When using concentrated chemicals always make sure that there is adequate ventilation. Always use appropriate chemical resistant gloves to protect your hands and skin and always wear eye protection such as chemical goggles. Do not eat, drink, or smoke where chemicals are handled, processed, or stored. Wash hands and skin following contact. If the substance gets into your eyes, rinse eyes thoroughly for at least 15 minutes with tap water and seek medical attention. For specific advice please consult the corresponding (Material) Safety Data Sheet of the substance.

All effluent releases that may include the substance must be directed to a (municipal) waste water treatment plant that removes the substance from the final releases to the receiving water.
Regulatory Information / Classification and Labeling

Under GHS substances are classified according to their physical, health, and environmental hazards. The hazards are communicated via specific labels and the (M)SDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemicals in use.

*Note:* The hazard statements and symbols presented here refer to the hazard properties of the concentrated substance and are meant to provide a brief overview of the substance’s labeling. It is not intended to be comprehensive or to replace information found in the (M)SDS.

**Labeling according to UN GHS**

UN GHS is the basis for country specific GHS labeling

![Signal word: Danger](image)

**Hazard statements:**

- H303: May be harmful if swallowed.
- H314: Causes severe skin burns and eye damage.
- H317: May cause an allergic skin reaction.
- H330: Fatal if inhaled.
- H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled.
- H335: May cause respiratory irritation.
- H401: Toxic to aquatic life.
- H411: Toxic to aquatic life with long lasting effects.

**Additional information**

1. IFA GESTIS-database on hazardous substances
2. Information on registered substance (ECHA)

3. BASF Basonat® Brochure
   http://www2.basf.us/rawmaterials/pdfs/Basonat.pdf

Most commonly used synonyms

» Cyclohexane, 5-isocyanato-1(isocyanatomethyl)-1,3,3-trimethyl-
» 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate

Disclaimer

This Product Safety Summary is intended to provide a general overview of the chemical substance. It contains basic information and is not intended to provide emergency response information, medical information or treatment information. The summary cannot be relied on to provide in-depth safety and health information. In-depth safety and health information must be obtained from the Material Safety Data Sheet ((M)SDS) for the chemical substance.

IMPORTANT: While the data and information contained herein are presented in good faith and believed to be accurate at the date of printing, it is provided for your guidance only and may be revised in the future. No warranties of any kind, either express or implied, of merchantability, fitness for a particular purpose or of any other nature are made regarding the data or information provided. Further, it is expressly understood that the data and information furnished by BASF hereunder are given gratis and BASF assumes no obligation or liability whatsoever resulting from use of or reliance on the data and information given.

Contact

For further information on this substance or GPS safety summaries in general, please contact:
info.gps@basf.com