SAFETY DATA SHEET
according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 12/13/2013
Version 1.0

SECTION 1. Identification

Product identifier

Product number  841355
Product name  Isophthalonitrile for synthesis
CAS-No.  626-17-5

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

Identified uses  Chemical for synthesis

Details of the supplier of the safety data sheet

Company  EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)

Emergency telephone  800-424-9300 CHEMTREC (USA)
+1-703-527-3887 CHEMTREC (International)
24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS-Labeling
Not a hazardous substance or mixture according to Regulation (EC) No 1272/2008.

OSHA Hazards
This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS and may deviate from the GHS information.

Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula  C₈H₄N₂ (Hill)
Molar mass  128.13 g/mol

Hazardous ingredients

Chemical Name (Concentration)
CAS-No.
SECTION 4. First aid measures

Description of first-aid measures

_Inhalation_
After inhalation: fresh air.

_Skin contact_
After skin contact: wash off with plenty of water. Remove contaminated clothing.

_Eye contact_
After eye contact: rinse out with plenty of water.

_Ingestion_
After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed
The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

_Suitable extinguishing media_
Water, Foam, Carbon dioxide (CO2), Dry powder

_Unsuitable extinguishing media_
For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture
Combustible.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapors possible in the event of fire.
Fire may cause evolution of:
Hydrogen cyanide (hydrocyanic acid)
Ammonia
nitrogen oxides

Advice for firefighters
_Special protective equipment for fire-fighters_
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

_Further information_
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

<table>
<thead>
<tr>
<th>Ingredients</th>
<th>Basis</th>
<th>Value</th>
<th>Threshold limits</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene-1,3-dicarbonitrile 626-17-5</td>
<td>ACGIH Time Weighted Average (TWA):</td>
<td>5 mg/m³</td>
<td>Form of exposure: Inhalable fraction and vapor.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NIOSH/GUIDE Recommended exposure limit (REL):</td>
<td>5 mg/m³</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Z1A Time Weighted Average (TWA):</td>
<td>5 mg/m³</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.
**Eye/face protection**
Safety glasses

**Hand protection**
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

**Respiratory protection**
required when dusts are generated.
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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**SECTION 9. Physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>powder</td>
</tr>
<tr>
<td>Color</td>
<td>white</td>
</tr>
<tr>
<td>Odor</td>
<td>bitter almond-like</td>
</tr>
<tr>
<td>Odor Threshold</td>
<td>No information available.</td>
</tr>
<tr>
<td>pH</td>
<td>No information available.</td>
</tr>
<tr>
<td>Melting point</td>
<td>162 - 163 °C</td>
</tr>
<tr>
<td>Boiling point/boiling range</td>
<td>550 °F (288 °C) at 1,013 hPa</td>
</tr>
<tr>
<td>Flash point</td>
<td>No information available.</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No information available.</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No information available.</td>
</tr>
<tr>
<td>Lower explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Upper explosion limit</td>
<td>No information available.</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>0.014 hPa at 68 °F (20 °C)</td>
</tr>
<tr>
<td></td>
<td>1.33 hPa at 190 °F (88 °C)</td>
</tr>
<tr>
<td></td>
<td>13 hPa at 279 °F (137 °C)</td>
</tr>
<tr>
<td>Relative vapor density</td>
<td>No information available.</td>
</tr>
</tbody>
</table>
Density
1.3 g/cm³
at 68 °F (20 °C)

Relative density
No information available.

Water solubility
0.7 g/l
at 68 °F (20 °C)

Partition coefficient: n-octanol/water
log Pow: 0.39
No information available.

Bioaccumulation is not expected. (External MSDS)

Autoignition temperature
No information available.

Decomposition temperature
No information available.

Viscosity, dynamic
No information available.

Explosive properties
Not classified as explosive.

Oxidizing properties
none

Bulk density
500 kg/m³

SECTION 10. Stability and reactivity

Reactivity
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents, Strong acids, strong alkalis, strong reducing agents

Conditions to avoid
Strong heating.

Incompatible materials
no information available

Hazardous decomposition products
in the event of fire: See section 5.
SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Inhalation, Eye contact, Skin contact, Ingestion

Target Organs
Eyes
Skin
Central nervous system

Acute oral toxicity
LD50 rat: > 2,000 mg/kg (External MSDS)

Acute inhalation toxicity
LC0 rat: 2.243 mg/l; 4 h (External MSDS)

Symptoms: Shortness of breath

Acute dermal toxicity
LD50 rabbit: > 2,000 mg/kg
(RTECS)

Skin irritation
rabbit
Result: No irritation
(External MSDS)

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC
No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

OSHA
No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

NTP
No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

ACGIH
No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
Further information
Possible symptoms:
Headache, Nausea, confusion, Unconsciousness
The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.
Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity
Toxicity to fish
LC50 Cyprinus carpio (Carp): 314 - 363 mg/l; 96 h (External MSDS)

Toxicity to bacteria
EC10 Pseudomonas putida: 180 mg/l(External MSDS)

Persistence and degradability
Biodegradability
OECD Test Guideline 301B
Not readily biodegradable.

Bioaccumulative potential
Partition coefficient: n-octanol/water
log Pow: 0.39
No information available.
Bioaccumulation is not expected. (External MSDS)

Mobility in soil
No information available.

Additional ecological information
Bactericidal effect. Discharge into the environment must be avoided.

SECTION 13. Disposal considerations
The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.
SECTION 14. Transport information

Land transport (DOT)
- UN number: UN 2811
- Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (ISOPHTHALONITRILE)
- Class: 6.1
- Packing group: II
- Environmentally hazardous: --

Air transport (IATA)
- UN number: UN 2811
- Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (ISOPHTHALONITRILE)
- Class: 6.1
- Packing group: II
- Environmentally hazardous: --
- Special precautions for user: no

Sea transport (IMDG)
- UN number: UN 2811
- Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (ISOPHTHALONITRILE)
- Class: 6.1
- Packing group: II
- Environmentally hazardous: --
- Special precautions for user: yes
- EmS: F-A S-A

SECTION 15. Regulatory information

United States of America

OSHA Hazards
- Target organ effects: Toxic by inhalation.

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards
- Acute Health Hazard
- Chronic Health Hazard

SARA 313
- SARA 313: 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 302
- SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.
DEA List I
Not listed

DEA List II
Not listed

US State Regulations

Massachusetts Right To Know
Ingredients
Benzene-1,3-dicarbonitrile

Pennsylvania Right To Know
Ingredients
Benzene-1,3-dicarbonitrile

New Jersey Right To Know
Ingredients
Benzene-1,3-dicarbonitrile

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

Notification status
TSCA: All components of the product are listed in the TSCA-inventory.
DSL: This product contains one or several components listed in the Canadian NDSL.

SECTION 16. Other information

Training advice
Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Date of issue: 12/13/2013

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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