



MATERIAL SAFETY DATA SHEET

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

Revision Date 08/20/2013

Version 1.1

SECTION 1. Identification

Product identifier

Product number	800593
Product name	Phthalonitrile for synthesis

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

Identified uses	Intermediate for use under strictly controlled conditions, Chemical for synthesis
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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)
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Acute toxicity, Category 3, Oral, H301

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

GHS-Labeling

Hazard pictograms



Signal Word

Danger

Hazard Statements

H301 Toxic if swallowed.

Precautionary Statements

P260 Do not breathe dust.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

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OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$C_6H_4-1,2-(CN)_2$	$C_8H_4N_2$ (Hill)
CAS-No.	91-15-6	
Molar mass	128.13 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

phthalonitrile (>= 90 % - <= 100 %)

91-15-6

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

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

Unconsciousness, Convulsions

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, Carbon dioxide (CO₂), Foam, Dry powder

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Unsuitable extinguishing media

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

Special hazards arising from the substance or mixture

Combustible material

Risk of dust explosion.

Development of hazardous combustion gases or vapors possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

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 substance contact. Ensure adequate ventilation.

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 empty into 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

Dry. Tightly closed. 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

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

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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. Work under hood. Do not inhale substance/mixture.

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.

Other protective equipment:

protective clothing

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.

SECTION 9. Physical and chemical properties

Physical state	powder, finecrystalline
Color	beige
Odor	odorless
Odor Threshold	not applicable
pH	7
Melting point	138 - 141 °C
Boiling point	No information available.
Flash point	> 266 °F (> 130 °C)
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.

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Vapor pressure	0.04 hPa at 68 °F (20 °C)
Relative vapor density	No information available.
Relative density	1.24 g/cm ³ at 68 °F (20 °C)
Water solubility	0.56 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 0.582 (25 °C) Bioaccumulation is not expected (log Pow <1). (External MSDS)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	> 1076 °F (> 580 °C)
Bulk density	500 kg/m ³

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

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

Sensitive to air.

Possibility of hazardous reactions

Exothermic reaction with:

Strong oxidizing agents, strong reducing agents, Strong acids and strong bases

Conditions to avoid

no information available

Incompatible materials

no information available

Hazardous decomposition products

in the event of fire: See section 5.

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SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 85 mg/kg

absorption

Skin irritation

rabbit

Result: No irritation
(External MSDS)

Eye irritation

rabbit

Result: No eye irritation
(External MSDS)

Genotoxicity in vitro

Ames test

Result: negative
(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

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Systemic effects:

After absorption:

Convulsions, Unconsciousness

Symptoms may be delayed.

Other information

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.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 *Oryzias latipes* (Orange-red killifish): 27 mg/l; 48 h (External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia magna* (Water flea): 219 mg/l; 48 h (External MSDS)

Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): 415 mg/l; 96 h (External MSDS)

Toxicity to bacteria

EC50 *Pseudomonas putida*: 211 mg/l; 17 h (External MSDS)

Persistence and degradability

Biodegradability

> 70 %

(External MSDS)

Not readily biodegradable.

Biochemical Oxygen Demand (BOD)

< 10 mg/g (5 d)

(External MSDS)

Chemical Oxygen Demand (COD)

1,015 mg/g

(External MSDS)

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0.582 (25 °C)

Bioaccumulation is not expected (log Pow <1). (External MSDS)

Mobility in soil

No information available.

Additional ecological information

Biological effects:

When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected.

Further information on ecology

Discharge into the environment must be avoided.

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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 3439
Proper shipping name NITRILES, TOXIC, SOLID, N.O.S. (PHTHALONITRILE)
Class 6.1
Packing group III
Environmentally hazardous --

Air transport (IATA)

UN number UN 3439
Proper shipping name NITRILES, SOLID, TOXIC, N.O.S. (PHTHALONITRILE)
Class 6.1
Packing group III
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 3439
Proper shipping name NITRILES, TOXIC, SOLID, N.O.S. (PHTHALONITRILE)
Class 6.1
Packing group III
Environmentally hazardous --
Special precautions for user yes
EmS F-A S-A

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Toxic by ingestion

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

SARA 313

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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.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

Ingredients

phthalonitrile

New Jersey Right To Know

Ingredients

phthalonitrile

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.
Ingredients
o-toluenitrile

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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

H301 Toxic if swallowed.

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.

Revision Date 08/20/2013

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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