



MATERIAL SAFETY DATA SHEET

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

Date of issue: 03/11/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number	816101
Product name	4,5-Dicyanoimidazole for synthesis

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

Identified uses	Use restricted under TSCA to research and development or as analytical reagent. Uses regulated under FDA or FIFRA are not affected. 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) e-mail: mm_sds@merckgroup.com
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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 4, Oral, H302

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

GHS-Labeling

Hazard pictograms



Signal Word
Warning

Hazard Statements
H302 Harmful if swallowed.

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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 $C_5H_2N_4$ (Hill)
CAS-No. 1122-28-7
Molar mass 118.1 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

4,5-dicyanoimidazole ($\geq 90\%$ - $\leq 100\%$)
1122-28-7

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: immediately make victim drink water (two glasses at most). Consult a physician.

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, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

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

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Special hazards arising from the substance or mixture

Combustible.

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

Fire may cause evolution of:

Hydrogen cyanide (hydrocyanic acid), 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

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Suppress (knock down) gases/vapors/mists with a water spray jet.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts.

Ensure adequate ventilation. 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

Tightly closed. Dry.

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

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.

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Hygiene measures

Change contaminated clothing. Application of skin- protective barrier cream recommended.
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.

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	crystalline
Color	white
Odor	No strong odor known.
Odor Threshold	No information available.
pH	No information available.
Melting point	171 - 175 °C
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	No information available.
Relative vapor density	No information available.
Relative density	No information available.

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Water solubility	slightly soluble
Partition coefficient: n-octanol/water	log Pow: -0.85 (calculated) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.

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

heat-sensitive

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Generates dangerous gases or fumes in contact with:

Acids

Conditions to avoid

no information available

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

Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 600 mg/kg (External MSDS)

absorption

Symptoms: We have no description of any toxic symptoms.

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Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(Lit.)

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

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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

No information available.

Persistence and degradability

No information available.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -0.85

(calculated)

(Lit.) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

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No information available.

Other adverse effects

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)

Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)

Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Harmful if swallowed.

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

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.

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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

Massachusetts Right To Know

Remarks

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

Pennsylvania Right To Know

Ingredients

4,5-dicyanoimidazole

New Jersey Right To Know

Ingredients

4,5-dicyanoimidazole

Notification status

TSCA:

Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.

Ingredients

4,5-dicyanoimidazole

DSL:

This product contains one or several components that are not on the Canadian DSL nor NDSL.

Ingredients

4,5-dicyanoimidazole

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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

H302

Harmful 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.

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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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