

SAFETY DATA SHEET

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

Revision Date 01/27/2015

Version 1.3

SECTION 1. Identification

Product identifier

Product number	840036
Product name	Cyanoacetone sodium salt for synthesis
CAS-No.	70807-22-6

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

Identified uses	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 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
Skin corrosion, Category 1B, H314
Serious eye damage, Category 1, H318
Skin sensitization, Category 1, H317

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.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.

Precautionary Statements

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P260 Do not breathe dust or mist.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P272 Contaminated work clothing should not be allowed out of the workplace.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 Immediately call a POISON CENTER or doctor/ physician.
P321 Specific treatment (see supplemental first aid instructions on this label).
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	C ₄ H ₄ ONNa (Hill)
Molar mass	105.07 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

3-oxo-butanenitrile sodium salt (>= 90 % - <= 100 %)

70807-22-6

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Call in physician.

Skin contact

After skin contact: wash off with plenty of water. Immediately remove contaminated clothing. If available swab with polyethylene glycol 400. Call a physician immediately.

Eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

Ingestion

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation!). Call a physician immediately. Do not attempt to neutralize.

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Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

Allergic reactions, Irritation and corrosion, Risk of blindness!

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.

Special hazards arising from the substance or mixture

Combustible material

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

Fire may cause evolution of:
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.

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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 +2°C to +8°C (+36°F to +46°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.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

Eye/face protection

Tightly fitting safety goggles

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:

Acid-resistant 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
Color	yellow
Odor	ammoniacal
Odor Threshold	No information available.

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pH	10.9 - 11.4 at 68 °F (20 °C) (saturated aqueous solution)
Melting point	ca. 240 °C (decomposition)
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	0.000016 hPa at 77 °F (25 °C)
Relative vapor density	No information available.
Density	1.17 g/cm ³ at 68 °F (20 °C)
Relative density	No information available.
Water solubility	460 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 0.5 (32 °C) (External MSDS) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none
Ignition temperature	1157 °F (625 °C)

SECTION 10. Stability and reactivity**Reactivity**

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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 moisture

Possibility of hazardous reactions

Violent reactions possible with:
Oxidizing agents, 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

Inhalation, Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 Rat: > 200 - 2,000 mg/kg

OECD Test Guideline 401

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

absorption

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Skin irritation

Rabbit

Result: Causes burns.

OECD Test Guideline 404

Causes burns.

Eye irritation

Causes serious eye damage.

Risk of blindness!

Sensitization

Sensitization test: Guinea pig

Result: positive

Method: OECD Test Guideline 406

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May cause an allergic skin reaction.

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

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.

This substance should be handled with particular care.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Danio rerio (zebra fish): 17 mg/l; 96 h

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 15 mg/l; 48 h

OECD Test Guideline 202

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Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): 2.4 mg/l; 72 h
OECD Test Guideline 201

Toxicity to bacteria

EC50 *Pseudomonas putida*: 7.4 mg/l; 16 h (External MSDS)

Persistence and degradability

Biodegradability

98 %; 28 d
OECD Test Guideline 301B
Readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0.5 (32 °C)
(External MSDS) Bioaccumulation is not expected.

Mobility in soil

No information available.

Additional ecological information

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 3263
Proper shipping name	CORROSIVE SOLID, BASIC, ORGANIC, N.O.S. (CYANOACETONE SODIUM SALT)
Class	8
Packing group	II
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 3263
Proper shipping name	CORROSIVE SOLID, BASIC, ORGANIC, N.O.S. (CYANOACETONE SODIUM SALT)
Class	8
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

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UN number	UN 3263
Proper shipping name	CORROSIVE SOLID, BASIC, ORGANIC, N.O.S. (CYANOACETONE SODIUM SALT)
Class	8
Packing group	II
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-B

SECTION 15. Regulatory information

United States of America

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

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.

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.

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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.

Labeling

Hazard pictograms



Signal Word

Danger

Hazard Statements

H301 Toxic if swallowed.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.

Precautionary Statements

Prevention

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Caution - substance not yet tested completely.

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

H301 Toxic if swallowed.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.

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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