

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 09.12.2015

Version 7.7

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No.	807068
Product name	Propionitrile for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	107-12-0

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225
Acute toxicity, Category 2, Oral, H300
Acute toxicity, Category 1, Dermal, H310
Acute toxicity, Category 4, Inhalation, H332
Eye irritation, Category 2, H319

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

Classification (67/548/EEC or 1999/45/EC)

F	Highly flammable	R11
T+	Very toxic	R27
T	Toxic	R25
Xn	Harmful	R20
Xi	Irritant	R36

For the full text of the R-phrases mentioned in this Section, see Section 16.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word
Danger

Hazard statements

H225 Highly flammable liquid and vapour.
H300 Fatal if swallowed.
H310 Fatal in contact with skin.
H319 Causes serious eye irritation.
H332 Harmful if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P280 Wear protective gloves/ protective clothing.

Response

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.

Storage

P403 + P235 Store in a well-ventilated place. Keep cool.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word
Danger

Hazard statements

H300 Fatal if swallowed.
H310 Fatal in contact with skin.

Precautionary statements

P280 Wear protective gloves/ protective clothing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 107-12-0

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

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Formula $\text{CH}_3\text{CH}_2\text{CN}$ $\text{C}_3\text{H}_5\text{N}$ (Hill)
EC-No. 203-464-4
Molar mass 55,08 g/mol

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
propionitrile ($\leq 100\%$)		
107-12-0	*)	

Flammable liquid, Category 2, H225
Acute toxicity, Category 2, H300
Acute toxicity, Category 4, H332
Acute toxicity, Category 1, H310
Eye irritation, Category 2, H319

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
propionitrile ($\leq 100\%$)	
107-12-0	F, Highly flammable; R11 T+, Very toxic; R27 T, Toxic; R25 Xn, Harmful; R20 Xi, Irritant; R36

For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration.
Oxygen if necessary. Immediately call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

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

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.

4.2 Most important symptoms and effects, both acute and delayed

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Shortness of breath, respiratory arrest, cardiovascular disorders, Convulsions, restlessness, death

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.
irritant effects

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Combustible.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Special protective equipment for firefighters

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

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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 carefully with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

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Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

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

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 mm

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Break through time: > 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 720 Camapren® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	ether-like
Odour Threshold	No information available.
pH	10 at 50 g/l 20 °C
Melting point	-92 °C
Boiling point/boiling range	97 °C at 1.013 hPa
Flash point	12 °C Method: DIN 51755 Part 1
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	3,1 %(V)

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Upper explosion limit	14 %(V)
Vapour pressure	50 hPa at 20 °C
Relative vapour density	No information available.
Density	0,782 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	103 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 0,16 (experimental) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0,44 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Ignition temperature	515 °C Method: DIN 51794
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SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Oxidizing agents

Violent reactions possible with:

Strong acids, strong alkalis, strong reducing agents

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

no information available

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10.6 Hazardous decomposition products
in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 39 mg/kg

(External MSDS)

Symptoms: Shortness of breath
absorption

Acute inhalation toxicity

LC50 Rat: 3,3 mg/l; 4 h ; vapour

(External MSDS)

Symptoms: Shortness of breath, Possible damages:, mucosal irritations
absorption

Acute dermal toxicity

LD50 Rabbit: 40 - 56 mg/kg

(External MSDS)

absorption

Skin irritation

Rabbit

Result: slight irritation

(RTECS)

Eye irritation

Rabbit

Result: Eye irritation

(RTECS)

Causes serious eye irritation.

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Result: negative

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

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Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Systemic effects:

After absorption:

rise in blood pressure, cardiovascular disorders, Convulsions, restlessness, respiratory arrest, death

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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 1.520 mg/l; 96 h
(External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 250 mg/l; 48 h
(External MSDS)

12.2 Persistence and degradability

Biochemical Oxygen Demand (BOD)

1.500 mg/g (5 d)

Chemical Oxygen Demand (COD)

2.040 mg/g

Ratio BOD/ThBOD

Biochemical Oxygen Demand (BOD) > 70 %

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,16

(experimental)

Bioaccumulation is not expected. (Lit.)

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 2404
14.2 Proper shipping name	PROPIONITRILE
14.3 Class	3 (6.1)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 2404
14.2 Proper shipping name	PROPIONITRILE
14.3 Class	3 (6.1)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes Not permitted for transport

Sea transport (IMDG)

14.1 UN number	UN 2404
14.2 Proper shipping name	PROPIONITRILE
14.3 Class	3 (6.1)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

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Major Accident Hazard Legislation	SEVESO III ACUTE TOXIC H1 Quantity 1: 5 t Quantity 2: 20 t SEVESO III FLAMMABLE LIQUIDS P5c Quantity 1: 5.000 t Quantity 2: 50.000 t
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
Substances of very high concern (SVHC)	This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).
<i>National legislation</i> Storage class	3

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

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

H225	Highly flammable liquid and vapour.
H300	Fatal if swallowed.
H310	Fatal in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

Full text of R-phrases referred to under sections 2 and 3

R11	Highly flammable.
R20	Harmful by inhalation.
R25	Toxic if swallowed.
R27	Very toxic in contact with skin.
R36	Irritating to eyes.

Training advice

Provide adequate information, instruction and training for operators.

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Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.
H300 + H310 Fatal if swallowed or in contact with skin
H319 Causes serious eye irritation.
H332 Harmful if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P240 Ground/bond container and receiving equipment.
P280 Wear protective gloves/ protective clothing.



Response

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.

Storage



P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Labelling (67/548/EEC or 1999/45/EC)

<i>Symbol(s)</i>	 F  T+	Highly flammable Very toxic
<i>R-phrases(s)</i>	11-20-25-27-36	Highly flammable. Harmful by inhalation. Toxic if swallowed. Very toxic in contact with skin. Irritating to eyes.
<i>S-phrases(s)</i>	9-16-28-36/37-45	Keep container in a well-ventilated place. Keep away from sources of ignition - No smoking. After contact with skin, wash immediately with plenty of soap and water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

EC-No. 203-464-4

Reduced labelling (≤125 ml)

<i>Symbol(s)</i>	 F  T+	Highly flammable Very toxic
<i>R-phrases(s)</i>	20-25-27	Harmful by inhalation. Toxic if swallowed. Very toxic in contact with skin.
<i>S-phrases(s)</i>	28-36/37-45	After contact with skin, wash immediately with plenty of soap and water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Key or legend to abbreviations and acronyms used in the safety data sheet

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Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.