

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 22.03.2018

Version 8.2

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

### 1.1 Product identifier

Catalogue No. 804805

Product name Isobutyronitrile 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. 78-82-0

### 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](http://www.merckgroup.com)).

### 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](mailto: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

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Catalogue No.	804805
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## Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225

Acute toxicity, Category 2, Inhalation, H330

Acute toxicity, Category 2, Dermal, H310

Acute toxicity, Category 2, Oral, H300

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

## 2.2 Label elements

### Labelling (REGULATION (EC) No 1272/2008)

#### *Hazard pictograms*



#### *Signal word*

Danger

#### *Hazard statements*

H225 Highly flammable liquid and vapour.

H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.

#### *Precautionary statements*

##### Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P233 Keep container tightly closed.

P280 Wear protective gloves/ protective clothing.

##### Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

##### Storage

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

## Reduced labelling (≤125 ml)

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.

*Precautionary statements*

P280 Wear protective gloves/ protective clothing.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 78-82-0

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	(CH <sub>3</sub> ) <sub>2</sub> CHCN	C <sub>4</sub> H <sub>7</sub> N (Hill)
EC-No.	201-147-5	
Molar mass	69,11 g/mol	

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

*Chemical name (Concentration)*

CAS-No.	Registration number	Classification
isobutyronitrile (<= 100 % )		

78-82-0 \*)

Flammable liquid, Category 2, H225

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Acute toxicity, Category 2, H300

Acute toxicity, Category 2, H330

Acute toxicity, Category 2, H310

\*) 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.

## 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

#### *General advice*

First aider needs to protect himself.

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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. Remove contact lenses.

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

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.

Shortness of breath, Dizziness, Headache, Convulsions, muscular weakness, Tremors, confusion

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## 4.3 Indication of any immediate medical attention and special treatment needed

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Foam, Carbon dioxide (CO<sub>2</sub>), 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.

Pay attention to flashback.

Forms explosive mixtures with air at ambient temperatures.

Vapours are heavier than air and may spread along floors.

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

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

### 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.

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## 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.

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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. Chemizorb®). Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## 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.

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## 7.3 Specific end use(s)

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

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## 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:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 120 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 890 Vitoject® (splash contact).

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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](http://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.

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## **SECTION 9. Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

Form	liquid
Colour	colourless
Odour	bitter almond-like
Odour Threshold	No information available.
pH	No information available.
Melting point	-72 °C



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Boiling point	No information available.
Flash point	8 °C Method: closed cup
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,6 %(V)
Upper explosion limit	12,7 %(V)
Vapour pressure	43,5 hPa at 25 °C  133 hPa at 54,4 °C
Relative vapour density	2,4
Density	0,77 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	240 mg/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 0,46 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.

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Decomposition temperature	No information available.
Viscosity, dynamic	0,35 mPa.s at 75 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Ignition temperature	482 °C
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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

Violent reactions possible with:

Strong oxidizing agents, Strong acids, strong alkalis, strong reducing agents

### 10.4 Conditions to avoid

May readily catch fire after brief contact with a source of ignition.

Warming.

### 10.5 Incompatible materials

various plastics

### 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: 50 mg/kg

(RTECS)

#### *Acute inhalation toxicity*

LC50 Rat: 0,85 mg/l; 4 h ; vapour

(External MSDS)

#### *Acute dermal toxicity*

LD50 Rabbit: 200 mg/kg

(RTECS)

#### *Skin irritation*

This information is not available.

#### *Eye irritation*

This information is not available.

#### *Sensitisation*

This information is not available.

#### *Germ cell mutagenicity*

#### *Genotoxicity in vitro*

Ames test

Salmonella typhimurium

Result: negative

(National Toxicology Program)

#### *Carcinogenicity*

This information is not available.

#### *Reproductive toxicity*

This information is not available.

#### *Teratogenicity*

This information is not available.

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## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Aspiration hazard*

This information is not available.

### **11.2 Further information**

Systemic effects:

Shortness of breath, Headache, Dizziness, confusion, muscular weakness, vasodilation,  
Tremors, Convulsions

Damage to:

Liver

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.

This substance should be handled with particular care.

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## **SECTION 12. Ecological information**

### **12.1 Toxicity**

#### *Toxicity to fish*

LC50 Pimephales promelas (fathead minnow): > 102,1 mg/l; 96 h

(External MSDS)

LC50 Pimephales promelas (fathead minnow): 245 mg/l; 48 h

(External MSDS)

#### *Toxicity to daphnia and other aquatic invertebrates*

NOEC Daphnia magna (Water flea): 94,3 mg/l; 48 h

(External MSDS)

EC50 Daphnia magna (Water flea): > 94,3 mg/l; 48 h

(External MSDS)

### **12.2 Persistence and degradability**

No information available.

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## 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 0,46

(experimental)

(Lit.) Bioaccumulation is not expected.

## 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

*Additional ecological information*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

14.1 UN number	UN 2284
14.2 Proper shipping name	ISOBUTYRONITRILE
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)

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14.1 UN number	UN 2284
14.2 Proper shipping name	ISOBUTYRONITRILE
14.3 Class	3 (6.1)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

## Sea transport (IMDG)

14.1 UN number	UN 2284
14.2 Proper shipping name	ISOBUTYRONITRILE
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
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14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code  
Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard	SEVESO III
Legislation	ACUTE TOXIC
	H2
	Quantity 1: 50 t
	Quantity 2: 200 t

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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.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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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
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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).
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## National legislation

Storage class	3
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## 15.2 Chemical safety assessment

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

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## 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.
H330	Fatal if inhaled.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H225 Highly flammable liquid and vapour.  
H300 + H310 + H330 Fatal if swallowed, in contact with skin or 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.  
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.



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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.

## 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](http://www.wikipedia.org).

## Regional representation

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

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*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.*