

## Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)  
Classifications according to Regulation (EC) No 1272/2008.  
Printdate 23 Oct 2023

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product name:

4-(3-Indolyl)-butyric acid

### 1.1. Catalog No.:

688395

### 1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical  
uses: R&D

### 1.3. Uses advised against:

HPC Standards GmbH  
Am Wieseneck 7

04451 Cunnersdorf  
Deutschland

Tel. +49 34291 3372-36  
Fax. +49 34291 3372-39  
contact@hpc-standards.com

### 1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36  
This number is only available during office hours.

## 2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Flammable liquids (Category 2), H225

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Eye irritation (Category 2), H319

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

F Highly flammable R11

Xn Harmful R20/21/22

Xi Irritant R36

### 2.2. Label elements

#### 2.2.1. Pictogram



## 2.2.2.

Signal word Danger

Hazard statement(s)

Highly flammable liquid and vapour. Harmful if swallowed, in contact with skin or if inhaled. Causes serious eye irritation. Wear protective gloves and protective clothing. Wear eye or face protection. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Avoid breathing vapour. Do not eat, drink or smoke when using this product. IF INHALED: Call a POISON CENTER or doctor if you feel unwell. Dispose of contents and container in accordance with all local, regional, national and international regulations.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Methyl cyanide

ACN

Formula : C<sub>2</sub>H<sub>3</sub>N

Molecular Weight : 41,05 g/mol

CAS-No. : 75-05-8

EC-No. : 200-835-2

Index-No. : 608-001-00-3

Registration number : 01-2119471307-38-XXXX

Hazardous ingredients

Component Classification Concentration

Acetonitrile

CAS-No.

EC-No.

Index-No.

Registration number

75-05-8

200-835-2

608-001-00-3

01-2119471307-38-XXXX

Flam. Liq. 2; Acute Tox. 4; Eye

Irrit. 2; H225, H302 + H312 +

H332, H319

<= 100 %

Hazardous ingredients

Component Classification Concentration

Acetonitrile

CAS-No.

EC-No.

Index-No.

Registration number

75-05-8

200-835-2

608-001-00-3

01-2119471307-38-XXXX

F, Xn, R11 - R20/21/22 - R36 <= 100 %

### 3.1.1. Formula

C<sub>12</sub>H<sub>13</sub>NO<sub>2</sub>

### 3.1.2. Molecular Weight (g/mol)

203.24

### 3.1.3. CAS-No.

133-32-4

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

no data available

## 5. FIRE-FIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

no data available

### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

## 6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures  
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.  
For personal protection see section 8.

6.2 Environmental precautions  
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up  
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections  
For disposal see section 13.

## 7. HANDLING AND STORAGE

7.1 Precautions for safe handling  
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

7.2 Conditions for safe storage, including any incompatibilities  
Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.  
Recommended storage temperature: 2 - 8 °C

7.3 Specific end uses  
no data available

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters  
Components with workplace control parameters  
Derived No Effect Level (DNEL)  
Application Area Workers  
Exposure routes Inhalation  
Health effect Acute local effects, Acute systemic effects  
Value 68 mg/m<sup>3</sup>  
Application Area Workers  
Exposure routes Skin contact  
Health effect Long-term systemic effects  
Value 32,2mg/kg BW/d  
Application Area Workers  
Exposure routes Inhalation  
Health effect Long-term local effects, Long-term systemic effects  
Value 68 mg/m<sup>3</sup>  
Application Area Workers  
Exposure routes Inhalation  
Health effect Long-term local effects, Long-term systemic effects  
Value 68 mg/m<sup>3</sup>  
Application Area Consumers  
Exposure routes Inhalation  
Health effect Acute local effects  
Value 220 mg/m<sup>3</sup>  
Application Area Consumers  
Exposure routes Inhalation  
Health effect Acute systemic effects  
Value 22 mg/m<sup>3</sup>  
Application Area Consumers  
Exposure routes Inhalation  
Health effect Long-term systemic effects  
Value 4,8 mg/m<sup>3</sup>

**Predicted No Effect Concentration (PNEC)**

Compartment	Value
Water	10 mg/l
Soil	2,41 mg/kg
Marine water	1 mg/l
Fresh water	10 mg/l
Fresh water sediment	7,53 mg/kg
Onsite sewage treatment plant	32 mg/l

**8.2 Exposure controls**

**Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

**Personal protective equipment**

**Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN166(EU).

**Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing.. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a fullface respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**9. PHYSICAL AND CHEMICAL PROPERTIES**

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

a) Appearance Form: clear, liquid

Colour: colourless

b) Odour ether-like

c) Odour Threshold no data available

d) pH no data available

e) Melting point/freezing point

Melting point/range: -48 °C

f) Initial boiling point and boiling range

81 - 82 °C

g) Flash point 2,0 °C - closed cup

h) Evaporation rate 5,8

i) Flammability (solid, gas) no data available

j) Upper/lower

flammability or

explosive limits

Upper explosion limit: 16 %(V)

Lower explosion limit: 3 %(V)

k) Vapour pressure 73,18 hPa at 15 °C

121,44 hPa at 25 °C

413,23 hPa at 55 °C

98,64 hPa at 20 °C

l) Vapour density 1,42 - (Air = 1.0)

m) Relative density 0,786 g/mL at 25 °C

n) Water solubility completely soluble  
o) Partition coefficient: noctanol/  
water  
log Pow: -0,54 at 25 °C  
p) Auto-ignition  
temperature  
524,0 °C  
q) Decomposition  
temperature  
no data available  
r) Viscosity no data available  
s) Explosive properties Not explosive  
t) Oxidizing properties The substance or mixture is not classified as oxidizing.  
9.2 Other safety information  
Surface tension 29,0 mN/m at 20,0 °C  
Relative vapour density 1,42 - (Air = 1.0)

## 10. STABILITY AND REACTIVITY

10.1 Reactivity  
no data available  
10.2 Chemical stability  
no data available  
10.3 Possibility of hazardous reactions  
no data available  
10.4 Conditions to avoid  
Heat, flames and sparks. Extremes of temperature and direct sunlight.  
10.5 Incompatible materials  
acids, Bases, Oxidizing agents, Alkali metals  
10.6 Hazardous decomposition products  
Other decomposition products - no data available

## 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects  
Acute toxicity  
LD50 Oral - rat - male - 1.320 - 6.690 mg/kg  
LC50 Inhalation - mouse - 4 h - 3587 ppm  
(OECD Test Guideline 403)  
LC50 Inhalation - rat - 4 h - 26,8 mg/l  
LD50 Dermal - rabbit - male and female - > 2.000 mg/kg  
(OECD Test Guideline 402)  
Skin corrosion/irritation  
Skin - rabbit  
Result: No skin irritation  
(OECD Test Guideline 404)  
Serious eye damage/eye irritation  
Eyes - rabbit  
Result: Irritating to eyes.  
(OECD Test Guideline 405)  
Respiratory or skin sensitisation  
Buehler Test - guinea pig  
Did not cause sensitisation on laboratory animals.  
(OECD Test Guideline 406)  
Germ cell mutagenicity  
Hamster  
ovary  
Result: negative  
Mutation in mammalian somatic cells.  
Ames test

S. typhimurium

Result: Not mutagenic in Ames Test.

Hamster

ovary

Result: Equivocal evidence.

Sister chromatid exchange

Mutagenicity (micronucleus test)

mouse

Result: Positive results were obtained in some in vivo tests.

Carcinogenicity

No evidence of carcinogenicity in animal studies (when indicated)

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

Additional Information

RTECS: AL7700000

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions.,

The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea,

Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of

coordination, stupor, death

## 12. ECOLOGICAL INFORMATION

12.1 Toxicity

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

no data available

12.6 Other adverse effects

no data available

## 13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

#### 14. TRANSPORT INFORMATION

14.1 UN number  
ADR/RID: 1648 IMDG: 1648 IATA: 1648  
14.2 UN proper shipping name  
ADR/RID: ACETONITRILE  
IMDG: ACETONITRILE  
IATA: Acetonitrile  
14.3 Transport hazard class(es)  
ADR/RID: 3 IMDG: 3 IATA: 3  
14.4 Packaging group  
ADR/RID: II IMDG: II IATA: II  
14.5 Environmental hazards  
ADR/RID: no IMDG Marine Pollutant: no IATA: no  
14.6 Special precautions for user  
no data available

#### 15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of the regulation named on the first page of this SDS.  
15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture  
no data available  
15.2 Chemical Safety Assessment  
no data available

#### 16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide.  
The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. For lab use only!