Chemical Safety Data Sheet MSDS / SDS

BUTYRONITRILE

Revision Date: 2025-01-18 Revision Number: 1

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

Product identifier

Product name : BUTYRONITRILE

CBnumber : CB0436355

CAS : 109-74-0

EINECS Number : 203-700-6

Synonyms : butyronitrile,butanenitrile

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.

Uses advised against : none

Company Identification

Company : Chemicalbook

Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing

Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word Danger

Precautionary statements

P405 Store locked up.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

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

Hazard statements

H331 Toxic if inhaled

H311 Toxic in contact with skin

H301 Toxic if swalloed

H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name : BUTYRONITRILE

Synonyms : butyronitrile,butanenitrile

CAS : 109-74-0
EC number : 203-700-6
MF : C4H7N
MW : 69.11

SECTION 4: First aid measures

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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

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

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NOx) Combustible.

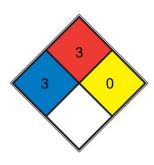
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704



Short exposure could cause serious temporary or moderate residual injury (e.g. <u>liquid hydrogen, sulfuric acid, calcium</u>

HEALTH 3

hypochlorite, hexafluorosilicic acid)

Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, acetone)

 $\begin{tabular}{lll} \blacksquare & REACT & 0 & Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, $\underline{N2}$) \\ \hline \end{tabular}$

SPEC.

FIRE

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, 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.

Environmental precautions

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

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

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.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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. Store in cool place.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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 EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's 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.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,3 mm Break through time: 480 min Material tested:Butoject? (KCL 897 / Aldrich Z677647, Size M)

Splash contact Material: butyl-rubber

Minimum layer thickness: 0,3 mm Break through time: 480 min Material tested:Butoject? (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

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 full- face 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.

Exposure limits

TLV-TWA 22.5 mg/m³ (8 ppm) (NIOSH).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Odour Threshold No data available PH No data available Melting point/freezing point Melting point/range: -112 °C - lit. Initial boiling point and boiling range 115 - 117 °C - lit. Flash point 22 °C - Regulation (EC) No. 440/2008, Annex, A.9 Evaporation rate No data available Flammability (solid, gas) No data available Flammability or explosive Lower explosion limit: 1,65 %(V) Ilimits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit. Water solubility 34,2 g/l at 20 °C - Regulation (EC) No. 440/2008, Annex, A.6
Melting point/freezing point Melting point/range: -112 °C - lit. Initial boiling point and boiling range 115 - 117 °C - lit. Flash point 22 °C - Regulation (EC) No. 440/2008, Annex, A.9 Evaporation rate No data available Flammability (solid, gas) No data available Upper/lower flammability or explosive Lower explosion limit: 1,65 %(V) Ilmits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Melting point/freezing point Melting point/range: -112 °C - lit. Initial boiling point and boiling range 115 - 117 °C - lit. Flash point 22 °C - Regulation (EC) No. 440/2008, Annex, A.9 Evaporation rate No data available Flammability (solid, gas) No data available Upper/lower flammability or explosive Ilimits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density Melting point/range: -112 °C - lit.
Initial boiling point and boiling range 115 - 117 °C - lit. Flash point 22 °C - Regulation (EC) No. 440/2008, Annex, A.9 Evaporation rate No data available Flammability (solid, gas) No data available Upper/lower flammability or explosive limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Flash point 22 °C - Regulation (EC) No. 440/2008, Annex, A.9 Evaporation rate No data available Flammability (solid, gas) No data available Upper/lower flammability or explosive Lower explosion limit: 1,65 %(V) limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Evaporation rate No data available Flammability (solid, gas) Upper/lower flammability or explosive Lower explosion limit: 1,65 %(V) limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Flammability (solid, gas) No data available Upper/lower flammability or explosive Lower explosion limit: 1,65 %(V) limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Upper/lower flammability or explosive Lower explosion limit: 1,65 %(V) limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
limits Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Vapour pressure 23 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4 Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Vapour density 2,39 - (Air = 1.0) Relative density 0,794 g/cm3 at 25 °C - lit.
Relative density 0,794 g/cm3 at 25 °C - lit.
Water solubility 34,2 g/l at 20 °C - Regulation (EC) No. 440/2008, Annex, A.6
Partition coefficient: n-octanol/water log Pow: 0,401 at 30 °C - Regulation (EC) No. 440/2008, Annex, A.8
Autoignition temperature No data available
Decomposition temperature No data available
Viscosity 0,555 mm2/s at 25 °C - OECD Test Guideline 114 -
Explosive properties No data available
Oxidizing properties No data available

Other safety information

Surface tension 23,7 mN/m at 100 at 21,1 °C

- Regulation (EC) No. 440/2008, Annex, A.5

Relative vapour density

2,39 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 50 - < 100 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Mouse - 4 h - 0,36 mg/l Remarks: (RTECS)

LD50 Dermal - Rabbit - 398 mg/kg Remarks: (RTECS)

Skin corrosion/irritation

Skin - Guinea pig

Result: slight irritation - 24 h Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation - 24 h (OECD Test Guideline 405) Eyes - Rabbit

Result: Mild eye irritation - 24 h

Respiratory or skin sensitisation

(OECD Test Guideline 429)

Germ cell mutagenicity

In vitro mammalian cell gene mutation test mouse lymphoma cells

Result: negative

Carcinogenicity

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

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rat - males - Oral - 90 d - No observed adverse effect level - 15 mg/kg

Repeated dose toxicity - Rat - females - Oral - 90 d - No observed adverse effect level - 25 mg/kg

RTECS: ET8750000

May cause cyanosis.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Toxicity

LD50 orally in rats: 0.14 g/kg (Smyth)

SECTION 12: Ecological information

Toxicity

Toxicity to fish

static test LC50 - Pimephales promelas (fathead minnow) - > 107

Toxicity to daphnia and other aquatic invertebrates

mg/l - 96 h

(OECD Test Guideline 203)

static test LC50 - Daphnia magna (Water flea) - > 110 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test EC50 - Pseudokirchneriella subcapitata (green algae) - > 133,4 mg/l - 72 h

(OECD Test Guideline 201)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 69 % - Readily biodegradable. (OECD Test Guideline 301D)

Remarks: The 10 day time window criterion is not fulfilled.

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Stability in water - > 1 yr at 25 °C at 50 °C< 10 % - 5 d (OECD Test Guideline 111)

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Waste Disposal

Burning in a chemical incinerator equipped with an afterburner and scrubber is the most effective way to destroy the compound. Oxidation with ethanolic–KOH can convert butyronitrile to nonhazardous cyanate.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2411 IMDG: 2411

UN proper shipping name

ADR/RID: BUTYRONITRILE IMDG: BUTYRONITRILE IATA: Butyronitrile

Transport hazard class(es)

ADR/RID: 3 (6.1) IMDG: 3 (6.1)

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

[1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

[2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

[3] ECHA - European Chemicals Agency, website: https://echa.europa.eu/

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

[6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

[7] HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

[8] IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

[9] IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

[10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Other Information

Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available. Depending on the degree of exposure, periodic medical examination is suggested.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.