Chemical Safety Data Sheet MSDS / SDS

Butyl isocyanate SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: Butyl isocyanate

CAS: 111-36-4

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.in

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SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 4, Oral

Skin corrosion, Sub-category 1B
Skin sensitization, Sub-category 1A
Serious eye damage, Category 1
Acute toxicity - Category 1, Inhalation
Specific target organ toxicity – single exposure, Category 3
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H302 Harmful if swallowed
H314 Causes severe skin burns and eye damage
H317 May cause an allergic skin reaction
H330 Fatal if inhaled
H335 May cause respiratory irritation
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P317 If skin irritation or rash occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P320 Specific treatment is urgent (see ... on this label).
P319 Get medical help if you feel unwell.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Butyl isocyanate
Common names and synonyms:	Butyl isocyanate
CAS number:	111-36-4
EC number:	203-862-8
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer immediately for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

Rinse with plenty of water for several minutes (remove contact lenses if easily possible).

Following ingestion

Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer immediately for medical attention.

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: TOXIC; inhalation, ingestion or contact (skin, eyes) with vapors, dusts or substance may cause severe injury, burns or death. Bromoacetates and chloroacetates are extremely irritating/lachrymators. Reaction with water or moist air will release toxic, corrosive or flammable gases. Reaction with water may generate much heat that will increase the concentration of fumes in the air. Fire will produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

Indication of immediate medical attention and special treatment needed, if necessary

Noncardiogenic pulmonary edema and bronchospasm are the most immediate serious clinical consequences of isocyanate exposure. Markedly symptomatic patients should receive oxygen, ventilatory support, and an intervenors line. Treatment for asthma includes inhaled sympathomimetics (salbutamol, metaproterenol), intravenous theophylline, parenteral sympathomimetics (epinephrine, terbutaline), and steroids. Isocyanates

SECTION 5: Firefighting measures

Suitable extinguishing media

Persons involved in fighting fires should wear a self-contained breathing apparatus with a full facepiece operated in a pressure-demand or other positive pressure mode. ... Methyl isocyanate

Specific hazards arising from the chemical

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapors may travel to source of ignition and flash back. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Substance will react with water (some violently) releasing flammable, toxic or corrosive gases and runoff. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated or if contaminated with water. (ERG, 2016)

Special protective actions for fire-fighters

Use dry powder, foam, carbon dioxide. NO water. In case of fire: keep drums, etc., cool by spraying with water. NO direct contact with water. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Ventilation. Remove all ignition sources. Personal protection: gas-tight chemical protection suit including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

Environmental precautions

Evacuate danger area! Ventilation. Remove all ignition sources. Personal protection: gas-tight chemical protection suit including

self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants and food and feedstuffs. Cool. See Chemical Dangers. Store in an area without drain or sewer access.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Butyl isocyanate			
CAS No.	111-36-4			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m^3	ppm	mg/m^3
Latvia	?	1	?	?
	Remarks			

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	N-butyl isocyanate is a clear, colorless liquid with a pungent odor. Very toxic by ingestion, and may also be toxic by skin absorption and inhalation. Vapors heavier than air. Less dense than water and insoluble in water. Produces toxic oxides of nitrogen during combustion.
Colour:	Colorless liquid
Odour:	no data available
Melting point/freezing point:	315°C(lit.)
Boiling point or initial boiling point and boiling range:	115°C
Flammability:	Highly flammable. Heating will cause rise in pressure with risk of bursting.

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	19°C(lit.)
Auto-ignition temperature:	425°C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water, 1.4X10+3 mg/L at 25 deg C (est)
Partition coefficient n-octanol/water:	log Kow = 2.26 (est)
Vapour pressure:	10.6 mm Hg (20 °C)
Density and/or relative density:	0.88
Relative vapour density:	3 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance may polymerize due to heating. Decomposes on burning. This produces toxic gases including nitrogen oxides and hydrogen cyanide. Reacts violently with strong oxidants and water.

Chemical stability

no data available

Possibility of hazardous reactions

The vapour mixes well with air, explosive mixtures are easily formed.Isocyanates and thioisocyanates are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidizers, hydrides, phenols, and peroxides can cause vigorous releases of heat. Acids and bases initiate polymerization reactions in these materials. Some isocyanates react with water to form amines and liberate carbon dioxide. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence [Wischmeyer 1969].

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

Energy of decomposition (in range 160 to 450 deg C) measured as 0.55 kJ/g.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Guinea pig oral 250 mg/kg

Inhalation: LC50 Rat inhalation 0.059 mg/L/4 hr 99.5% purity

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is corrosive to the eyes, skin and respiratory tract. Inhalation may cause lung oedema. See Notes.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. See Notes.

Aspiration hazard

A harmful contamination of the air will be reached quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

Isocyanates undergo rapid hydrolysis under environmental conditions with half-lives of less than 10 minutes(1). Therefore,

hydrolysis is expected to be the dominant fate process for n-butyl isocyanate in moist soil and water(SRC). Biodegradation is not expected to compete with hydrolysis as an important fate process(SRC).

Bioaccumulative potential

Isocyanates undergo rapid hydrolysis under environmental conditions with half-lives of less than 10 minutes(1). Therefore, hydrolysis is expected to be the dominant fate process for n-butyl isocyanate in water(SRC). Bioconcentration is not expected to compete with hydrolysis as an important environmental process(SRC).

Mobility in soil

Isocyanates undergo rapid hydrolysis under environmental conditions with half-lives of less than 10 minutes(1). Therefore, hydrolysis is expected to be the dominant fate process for n-butyl isocyanate in moist soil and water(SRC). Adsorption to soil and sediment is not expected to compete with hydrolysis as an important environmental process(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2485 (For reference only, please check.)
IMDG: UN2485 (For reference only, please check.)

IATA: UN2485 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: n-BUTYL ISOCYANATE (For reference only, please check.)
IMDG: n-BUTYL ISOCYANATE (For reference only, please check.)
IATA: n-BUTYL ISOCYANATE (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

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

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

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

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

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

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

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

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

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

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

Other Information

Some isocyanates are well known to cause respiratory sensitization. However, there are no reports of n-butyl isocyanate or other monoisocyanates causing respiratory sensitization. The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential.