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Safety data sheet

BASF Safety data sheet according to the United Nations' Globally Harmonized System (UN GHS)
Date / Revised: 01.09.2023 Version: 4.0
Product: **ISOBUTYRALDEHYDE**

(ID no. 30036664/SDS_GEN_00/EN)
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1. Identification

Product identifier

ISOBUTYRALDEHYDE

Chemical name: Isobutyraldehyde
CAS Number: 78-84-2

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

Relevant identified uses: Chemical

Details of the supplier of the safety data sheet

Company:
BASF SE
67056 Ludwigshafen
GERMANY
Operating Division Petrochemicals

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2. Hazards Identification

Classification of the substance or mixture

According to UN GHS criteria

Flam. Liq. 2

Acute Tox. 5 (oral)
Eye Dam./Irrit. 2B
Aquatic Acute 3

For the classifications not written out in full in this section the full text can be found in section 16.

Label elements

Globally Harmonized System (GHS)

Pictogram:

Signal Word:
Danger

Hazard Statement:

H225	Highly flammable liquid and vapour.
H320	Causes eye irritation.
H303	May be harmful if swallowed.
H402	Harmful to aquatic life.

Precautionary Statements (Prevention):

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280	Wear protective gloves and eye protection or face protection.
P243	Take action to prevent static discharges.
P273	Avoid release to the environment.
P241	Use explosion-proof electrical, ventilating and lighting equipment.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P242	Use non-sparking tools.
P264	Wash contaminated body parts thoroughly after handling.

Precautionary Statements (Response):

P312	Call a POISON CENTER or physician if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P337 + P311	If eye irritation persists: Call a POISON CENTER or physician.
P370 + P378	In case of fire: Use … to extinguish.

Precautionary Statements (Storage):

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

Precautionary Statements (Disposal):

P501	Dispose of contents and container to hazardous or special waste collection point.

Other hazards

According to UN GHS criteria

If applicable information is provided in this section on other hazards which do not result in classification but which may contribute to the overall hazards of the substance or mixture.

The product does not fulfill the criteria for PBT (Persistent/bioaccumulative/toxic) and vPvB (very persistent/very bioaccumulative).

3. Composition/Information on Ingredients

Substances

Chemical nature

Isobutyraldehyde
CAS Number: 78-84-2
EC-Number: 201-149-6

Hazardous ingredients (GHS)
According to UN GHS criteria

Isobutyraldehyde

Content (W/W): >= 99,2 % - <= 99,9 %	Flam. Liq. 2
CAS Number: 78-84-2	Acute Tox. 5 (oral)
EC-Number: 201-149-6	Eye Dam./Irrit. 2B
	Aquatic Acute 3
	H225, H320, H303, H402

For the classifications not written out in full in this section the full text can be found in section 16.

Mixtures

Not applicable

4. First-Aid Measures

Description of first aid measures

Immediately remove contaminated clothing. If the patient is likely to become unconscious, place and transport in stable sideways position (recovery position). If not breathing, give artificial respiration. First aid personnel should pay attention to their own safety.

If inhaled:
Keep patient calm, remove to fresh air, seek medical attention.

On skin contact:
Wash thoroughly with soap and water

On contact with eyes:

Wash affected eyes for at least 15 minutes under running water with eyelids held open. If irritation develops, seek medical attention.

On ingestion:
Rinse mouth and then drink 200-300 ml of water.

Most important symptoms and effects, both acute and delayed

Symptoms: Information, i.e. additional information on symptoms and effects may be included in the GHS labeling phrases available in Section 2 and in the Toxicological assessments available in Section 11.

Indication of any immediate medical attention and special treatment needed

Treatment: Treat according to symptoms (decontamination, vital functions), no known specific antidote.

5. Fire-Fighting Measures

Extinguishing media

Suitable extinguishing media:
dry powder, water spray, carbon dioxide, alcohol-resistant foam

Unsuitable extinguishing media for safety reasons:
water jet

Additional information:
Use extinguishing measures to suit surroundings.

Special hazards arising from the substance or mixture

Highly flammable. Cool endangered containers with water-spray. See SDS section 7 - Handling and storage.

Advice for fire-fighters

Special protective equipment:
Wear a self-contained breathing apparatus. Special protective equipment for firefighters

Further information:
Evacuate area of all unnecessary personnel. Fight fire from maximum distance.

Extend fire extinguishing measures to the surroundings. Dispose of fire debris and contaminated extinguishing water in accordance with official regulations.

6. Accidental Release Measures

High risk of slipping due to leakage/spillage of product.

Release of substance/product can cause fire or explosion. Shut off or stop source of leak. Shut off or stop released substance/product under safe conditions.

Pack in tightly closed containers for disposal.

Personal precautions, protective equipment and emergency procedures

Handle in accordance with good industrial hygiene and safety practice.

Avoid all sources of ignition: heat, sparks, open flame. Use antistatic tools.

Environmental precautions

Discharge into the environment must be avoided.

Methods and material for containment and cleaning up

Pick up with suitable appliance and dispose of. Spills should be contained, solidified, and placed in suitable containers for disposal. Dispose of absorbed material in accordance with regulations.

7. Handling and Storage

Precautions for safe handling

Handle in accordance with good industrial hygiene and safety practice.

Protection against fire and explosion:
Avoid all sources of ignition: heat, sparks, open flame. Ground all transfer equipment properly to prevent electrostatic discharge.

Conditions for safe storage, including any incompatibilities

Further information on storage conditions: Keep container tightly closed in a cool, well-ventilated place. Avoid all sources of ignition: heat, sparks, open flame.

Specific end use(s)

For the relevant identified use(s) listed in Section 1 the advice mentioned in this section 7 is to be observed.

8. Exposure Controls/Personal Protection

Control parameters

Components with occupational exposure limits

78-84-2: Isobutyraldehyde

Exposure controls

Personal protective equipment

Respiratory protection:
Wear respiratory protection if ventilation is inadequate. Gas filter for gases/vapours of organic compounds (boiling point <65 °C, f.e. EN 14387 Type AX)

Hand protection:
Chemical resistant protective gloves (EN ISO 374-1)
Suitable materials also with prolonged, direct contact (Recommended: Protective index 6, corresponding > 480 minutes of permeation time according to EN ISO 374-1):
butyl rubber (butyl) - 0.7 mm coating thickness
Manufacturer's directions for use should be observed because of great diversity of types.

Supplementary note: The specifications are based on tests, literature data and information of glove manufacturers or are derived from similar substances by analogy. Due to many conditions (e.g. temperature) it must be considered, that the practical usage of a chemical-protective glove in practice may be much shorter than the permeation time determined through testing.

Eye protection:
Safety glasses with side-shields (frame goggles) (e.g. EN 166)

Body protection:
Body protection must be chosen depending on activity and possible exposure, e.g. apron, protecting boots, chemical-protection suit (according to EN 14605 in case of splashes or EN ISO 13982 in case of dust).

General safety and hygiene measures
Avoid inhalation of vapour. Handle in accordance with good industrial hygiene and safety practice. Wearing of closed work clothing is required additionally to the stated personal protection equipment.

9. Physical and Chemical Properties

Information on basic physical and chemical properties

Form:	liquid	
Colour:	colourless	
Odour:	aldehyde-like	
Odour threshold:	not determined	
pH value:	not applicable	
Melting point:	-65,9 °C Literature data.	
Boiling point:	64 °C (1.013,25 hPa)	(measured)
Flash point:	-24 °C	(DIN 51755, closed cup)
Evaporation rate:	Value can be approximated from Henry's Law Constant or vapor pressure.	
Flammability:	Highly flammable.	(derived from flash - and boiling point)
Lower explosion limit:	For liquids not relevant for classification and labelling., The lower explosion point may be 5 - 15 °C below the flash point.	
Upper explosion limit:	For liquids not relevant for classification and labelling.	
Ignition temperature:	180 °C	(ASTM E659)
Vapour pressure:	189 mbar (20 °C) 0,6249 bar (50 °C)	
Density:	0,79 g/cm3 (20 °C)	

	0,7504 g/cm3 (55 °C)	(calculated)
Relative density:	0,78 (25,8 °C)	
Relative vapour density (air):	2,48 (20 °C) Heavier than air.	(calculated)
Solubility in water:	Literature data. 60 g/l (25 °C, 1.013,25 hPa)	
Partitioning coefficient n-octanol/water (log Kow):	0,77 (25 °C)	(OECD Guideline 107)
Self ignition:	Based on its structural properties the product is not classified as self-igniting.	Test type: Spontaneous self-ignition at room-temperature.
Thermal decomposition:	No decomposition if stored and handled as prescribed/indicated.	
Viscosity, dynamic:	0,43 mPa.s (20 °C) Literature data.	
Viscosity, kinematic:	No data available.	
Explosion hazard:	Based on the chemical structure there is no indication of explosive properties.	
Fire promoting properties:	Based on its structural properties the product is not classified as oxidizing.	

Other information

Self heating ability:	not applicable, the product is a liquid	
pKA:	The substance does not dissociate.	
Adsorption/water - soil:	KOC: 1,51; log KOC: 0,18	(calculated)
Surface tension:	Based on chemical structure, surface activity is not to be expected.	
Grain size distribution:	Test substance	The substance / product is marketed or used in a non solid or granular form.
Molar mass:	72,11 g/mol	

10. Stability and Reactivity

Reactivity

Corrosion to metals:	No corrosive effect on metal.	
Formation of flammable gases:	Remarks:	Forms no flammable gases in the presence of water.

Chemical stability

The product is stable if stored and handled as prescribed/indicated.

Possibility of hazardous reactions
When finely distributed, self-ignition is possible.

Conditions to avoid
Avoid all sources of ignition: heat, sparks, open flame.

Incompatible materials

Substances to avoid:
acids, bases, amines, oxidizing agents

Hazardous decomposition products

Hazardous decomposition products:
No hazardous decomposition products if stored and handled as prescribed/indicated.

11. Toxicological Information

Information on toxicological effects

Acute toxicity

Assessment of acute toxicity:
Of low toxicity after single ingestion. Virtually nontoxic by inhalation. Virtually nontoxic after a single skin contact.

Experimental/calculated data:
LD50 rat (oral): 3.730 mg/kg
An aqueous solution was tested.

LC50 rat (by inhalation): > 23,9 mg/l 4 h (similar to OECD guideline 403)
The vapour was tested.

LD50 rabbit (dermal): 5.583 mg/kg

Irritation

Assessment of irritating effects:
Not irritating to the skin. Eye contact causes irritation.

Experimental/calculated data:
Skin corrosion/irritation rabbit: non-irritant (OECD Guideline 404)

Serious eye damage/irritation rabbit: Irritant. (OECD Guideline 405)

Respiratory/Skin sensitization

Assessment of sensitization:
Skin sensitizing effects were not observed in animal studies.

Experimental/calculated data:
Mouse ear swelling test (MEST) mouse: Non-sensitizing.

Germ cell mutagenicity

Assessment of mutagenicity:
In the majority of studies performed with microorganisms and in mammalian cell culture, a mutagenic effect was not found. A mutagenic effect was also not observed in in vivo tests. The substance was not mutagenic in bacteria. The substance induced chromosomal aberrations in a mammalian cell culture test. The substance was not mutagenic in studies with mammals.

Carcinogenicity

Assessment of carcinogenicity:
In long-term studies in rats and mice in which the substance was given by inhalation, a carcinogenic effect was not observed.

Reproductive toxicity

Assessment of reproduction toxicity:
Repeated inhalative uptake of the substance did not cause damage to the reproductive organs. The results of animal studies gave no indication of a fertility impairing effect. The product has not been fully tested. The statements have been derived in parts from products of a similar structure or composition.

Developmental toxicity

Assessment of teratogenicity:
No indications of a developmental toxic / teratogenic effect were seen in animal studies.

Specific target organ toxicity (single exposure)

Assessment of STOT single:
Based on the available information there is no specific target organ toxicity to be expected after a single exposure.

Repeated dose toxicity and Specific target organ toxicity (repeated exposure)

Assessment of repeated dose toxicity:
The substance may cause damage to the upper respiratory tract after repeated inhalation, as shown in animal studies.

Aspiration hazard

No aspiration hazard expected.

12. Ecological Information

Toxicity

Assessment of aquatic toxicity:
Acutely harmful for aquatic organisms. The inhibition of the degradation activity of activated sludge is not anticipated when introduced to biological treatment plants in appropriate low concentrations.

Toxicity to fish:
LC50 (96 h) 23 mg/l, Pimephales promelas (APHA 1971, static)

Aquatic invertebrates:
EC50 (48 h) 277 mg/l, Daphnia magna (Directive 79/831/EEC, static)
The details of the toxic effect relate to the nominal concentration.

Aquatic plants:
EC50 (72 h) 83,7 mg/l (growth rate), Desmodesmus subspicatus (DIN 38412 Part 9, static)

Microorganisms/Effect on activated sludge:
No observed effect concentration (14 d) 100 mg/l, (Oxygen consumption test, aquatic)

EC50 (17 h) 468 mg/l, Pseudomonas putida (DIN 38412 Part 8, aquatic)

Chronic toxicity to fish:
No data available regarding toxicity to fish.

Chronic toxicity to aquatic invertebrates:
No data available regarding toxicity to daphnids.

Assessment of terrestrial toxicity:
No data available concerning terrestrial toxicity.

Persistence and degradability

Assessment biodegradation and elimination (H2O):
Readily biodegradable (according to OECD criteria).

Elimination information:
80 - 90 % BOD of the ThOD (14 d) (OECD 301C; ISO 9408; 92/69/EEC, C.4-F) (aerobic, Inoculum conforming to MITI requirements (OECD 301C))

Assessment of stability in water:
According to structural properties, hydrolysis is not expected/probable.
Information on Stability in Water (Hydrolysis):
No data available.

Bioaccumulative potential

Assessment bioaccumulation potential:
Significant accumulation in organisms is not to be expected.

Bioaccumulation potential:
No data available.

Mobility in soil

Assessment transport between environmental compartments:
Volatility: The substance will slowly evaporate into the atmosphere from the water surface.
Adsorption in soil: Adsorption to solid soil phase is not expected.

Results of PBT and vPvB assessment

According to Annex XIII of Regulation (EC) No.1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH): The product does not fulfill the criteria for PBT

(Persistent/bioaccumulative/toxic) and vPvB (very persistent/very bioaccumulative). Self classification

Other adverse effects

The substance is not listed in Regulation (EC) 1005/2009 on substances that deplete the ozone layer.

Additional information

Sum parameter

Chemical oxygen demand (COD): 1.992 mg/g

Adsorbable organically-bound halogen (AOX):
This product contains no organically-bound halogen.

13. Disposal Considerations

Waste treatment methods

Dispose of in accordance with national, state and local regulations.

Contaminated packaging:
Disposal must be made according to official regulations.

14. Transport Information

Land transport

ADR

UN number or ID number:	UN2045
UN proper shipping name:	ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
Transport hazard class(es):	3
Packing group:	II
Environmental hazards:	no
Special precautions for user:	Tunnel code: D/E

RID

UN number or ID number:	UN2045
UN proper shipping name:	ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
Transport hazard class(es):	3
Packing group:	II
Environmental hazards:	no
Special precautions for user:	None known

Inland waterway transport

ADN

UN number or ID number:	UN2045
UN proper shipping name:	ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
Transport hazard class(es):	3
Packing group:	II
Environmental hazards:	no
Special precautions for user:	None known

Transport in inland waterway vessel

UN number or ID number:	UN2045
UN proper shipping name:	ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
Transport hazard class(es):	3, N3
Packing group:	II
Environmental hazards:	yes
Type of inland waterway vessel:	C
Cargo tank design:	2
Cargo tank type:	2

Sea transport

IMDG

UN number or ID number:	UN 2045
UN proper shipping name:	ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
Transport hazard class(es):	3
Packing group:	II
Environmental hazards:	no Marine pollutant: NO
Special precautions for user:	EmS: F-E; S-D

Air transport

IATA/ICAO

UN number or ID number:	UN 2045
UN proper shipping name:	ISOBUTYRALDEHYDE
Transport hazard class(es):	3
Packing group:	II
Environmental hazards:	No Mark as dangerous for the environment is needed
Special precautions for user:	None known

Maritime transport in bulk according to IMO instruments

Regulation:	IBC-Code
Product name:	Butyraldehyde (all isomers)
Pollution category:	Y
Ship Type:	3

15. Regulatory Information

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

If other regulatory information applies that is not already provided elsewhere in this safety data sheet, then it is described in this subsection.

If other regulatory information applies that is not already provided elsewhere in this safety data sheet, then it is described in this subsection.

16. Other Information

Full text of classifications, hazard symbols and hazard statements, if mentioned in section 2 or 3:

Flam. Liq.	Flammable liquids
Acute Tox.	Acute toxicity
Eye Dam./Irrit.	Serious eye damage/eye irritation
Aquatic Acute	Hazardous to the aquatic environment - acute
H225	Highly flammable liquid and vapour.
H320	Causes eye irritation.
H303	May be harmful if swallowed.
H402	Harmful to aquatic life.

The data contained in this safety data sheet are based on our current knowledge and experience and describe the product only with regard to safety requirements. This safety data sheet is neither a Certificate of Analysis (CoA) nor technical data sheet and shall not be mistaken for a specification agreement. Identified uses in this safety data sheet do neither represent an agreement on the corresponding contractual quality of the substance/mixture nor a contractually designated use. It is the responsibility of the recipient of the product to ensure any proprietary rights and existing laws and legislation are observed.