

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision
Supersedes Version

5.01
5.00***

Revision Date
Issuing date

10-Feb-2021
10-Feb-2021

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

1.1. Product identifier

Identification of the
substance/preparation

Isobutyraldehyde

CAS-No 78-84-2
EC No. 201-149-6
Registration number (REACH) 01-2119456807-27

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

Identified uses Transported isolated intermediate (1907/2006)
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking
Identification

OQ Chemicals GmbH
Rheinpromenade 4A
D-40789 Monheim
Germany

OQ Chemicals Corporation
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number +65 3158 1198 (available 24/7)
000800 100 7479 (for domestic shipments only)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Flammable liquid Category 2, H225
Serious eye damage/eye irritation Category 2, H319

Additional information

For full text of Hazard- and EU Hazard-statements see SECTION 16.

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2.2. Label elements

Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).

Hazard pictograms



Signal word

Danger

Hazard statements

H225: Highly flammable liquid and vapour.
H319: Causes serious eye irritation.

Precautionary statements

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313: If eye irritation persists: Get medical advice/ attention.
P403 + P235: Store in a well ventilated place. Keep cool.

2.3. Other hazards

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback
Vapours may form explosive mixture with air
Auto ignition on large surfaces
Hazardous polymerisation may occur
Polymerization is a highly exothermic reaction and may generate sufficient heat to cause thermal decomposition and/or rupture containers
Components of the product may be absorbed into the body by inhalation and ingestion

PBT and vPvB assessment This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACH-No	1272/2008/EC	Concentration (%)
Isobutyraldehyde	78-84-2	01-2119456807-27	Flam. Liq. 2; H225 Eye Irrit. 2; H319	> 97

Remarks

Substance manufactured in Europe contains the following stabilizer(s):. Triethanolamine.
For full text of Hazard- and EU Hazard-statements see SECTION 16.

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SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.

Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion

Do not induce vomiting without medical advice. Call a physician immediately.

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

Main symptoms

shortness of breath, abdominal pain, circulatory collapse, cough.

Special hazard

Lung oedema, Lung irritation.

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

General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. In case of lung irritation, first treatment with cortisone spray. Symptoms may be delayed.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

alcohol-resistant foam, dry chemical, carbon dioxide (CO₂), water spray

Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO₂)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback

Vapours may form explosive mixture with air

5.3. Advice for firefighters

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Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting

Cool containers / tanks with water spray. Dike and collect water used to fight fire. Water run-off and vapor cloud may be corrosive. Keep people away from and upwind of fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.

For emergency responders: Personal protection see section 8.

6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant).

6.3. Methods and material for containment and cleaning up

Methods for containment

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up

Soak up with inert absorbent material. DO NOT use combustible materials such as sawdust. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms. Refill and handle product only in closed system. Do not use compressed air for filling, discharging or handling.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

acids and bases

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amines
oxidizing agents
reducing agents

7.2. Conditions for safe storage, including any incompatibilities

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback. Vapours may form explosive mixture with air. Hazardous polymerisation may occur. Polymerization is a highly exothermic reaction and may generate sufficient heat to cause thermal decomposition and/or rupture containers.

Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Handle under nitrogen, protect from moisture. Keep at temperatures between 15 and 33 °C (59 and 91 °F). Oxidization creates acids and peroxides, that may lead to corrosive damages in storage and handling equipment.

Suitable material

stainless steel, aluminium

Unsuitable material

mild steel

Temperature class

T4

7.3. Specific end use(s)

Transported isolated intermediate (1907/2006)

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits India

No exposure limits established.

8.2. Exposure controls

Appropriate Engineering controls

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures

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When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Respiratory protection

Respirator with AX filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	butyl-rubber
Evaluation	according to EN 374: level 3
Glove thickness	approx 0,3 mm
Break through time	approx 60 min
Suitable material	polyvinylchloride
Evaluation	Information derived from practical experience
Glove thickness	approx 0,8 mm

Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

Equipment should conform to EN 166

Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. Observe the exposure limits, clean exhaust air if needed. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	liquid
Colour	colourless
Odour	pungent
Odour threshold	0,2 mg/m ³
pH	No data available
Melting point/range	-65,9 °C
Boiling point/range	64,4 °C @ 1013 hPa
Flash point	-23 °C @ 1013 hPa***
Method	DIN 51755
Evaporation rate	9,6 (n-Butyl acetate = 1)
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	1,6 Vol %
Upper explosion limit	10,6 Vol %

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
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230	23	0,227	25	77
Vapour density		2,5 (Air = 1) @ 20 °C (68 °F)		
Relative density				
Values	@ °C	@ °F	Method	
0,78***	25,8***	78,4***	DIN 51757	
Solubility	60 g/l @ 25 °C, in water			
log Pow	0,77 @ 25 °C (77 °F), OECD 107***			
Autoignition temperature	180 °C @ 1013 hPa***			
Method	ASTM E 659			
Decomposition temperature	No data available			
Viscosity	0,43 mPa*s @ 20 °C			
Method	ISO 3219, dynamic***			
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties			
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties			

9.2. Other information

Molecular weight	72,11
Molecular formula	C4 H8 O
log Koc	0,18 @ 25°C (77 °F) calculated***
Refractive index	1,373 @ 20 °C
Heat of combustion	600 kcal/kg

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions. Stable up to approximately 49 °C.

10.3. Possibility of hazardous reactions

Hazardous reactions occur in the presence of acids, base or oxidizing agents. This reaction is exothermic and may create heat. When finely distributed, self-ignition is possible. May form explosive peroxides.***

10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

10.5. Incompatible materials

bases, amines, acids, oxidizing agents, reducing agents.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Ingestion, Inhalation, Eye contact, Skin contact

Acute toxicity				
Isobutyraldehyde (78-84-2)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	3730 mg/kg	rat, female***	OECD 401***
Dermal	LD50	5583 mg/kg	rabbit male***	Draize Test
Inhalative	LC50	> 23,6 mg/l (4h)	rat, male***	OECD 403***

Isobutyraldehyde, CAS: 78-84-2

Assessment

Based on available data, the classification criteria are not met for:

Acute oral toxicity
Acute dermal toxicity
Acute inhalation toxicity
STOT SE

Irritation and corrosion				
Isobutyraldehyde (78-84-2)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	No skin irritation	OECD 404	4h
Eyes	rabbit	irritating***	OECD 405	24h***
Respiratory tract***	mouse male***	RD50: 8,9 mg/l***		10 min***

Isobutyraldehyde, CAS: 78-84-2

Assessment

The available data lead to the classification given in section 2***

Sensitization				
Isobutyraldehyde (78-84-2)				
Target Organ Effects	Species	Evaluation	Method	
Skin	mouse female***	not sensitizing	MEST	3 - 30 % Substance

Isobutyraldehyde, CAS: 78-84-2

Assessment

Based on available data, the classification criteria are not met for:

Skin sensitization
For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity				
Isobutyraldehyde (78-84-2)				
Type	Dose	Species	Method	
Subchronic toxicity	NOAEL: > 1450 mg/kg/d***	rat, male/female mouse, male/female***	OECD 408***	Inhalation Oral read across***
Subchronic toxicity	NOAEC: 6 mg/l/d (13 weeks)***	mouse, male/female rat, male/female***	OECD 413	Inhalation

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Assessment

Based on available data, the classification criteria are not met for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Isobutyraldehyde (78-84-2)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		CHO (Chinese Hamster Ovary) cells	negative	OECD 476 (Mammalian Gene Mutation)	In vitro study
Mutagenicity		V79 cells, Chinese hamster	positive (without metabolic activation)	OECD 473 (Chromosomal Aberration)	In vitro study
Mutagenicity		Salmonella typhimurium Escherichia coli***	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		mouse male***	negative	Chromosomal Aberration	Bone marrow
Mutagenicity		rat male***	negative	Chromosomal Aberration	Bone marrow
Mutagenicity***		rat male***	negative***	OECD 489 Comet Assay***	In vitro study***
Reproductive toxicity	NOAEL: >= 7,5 mg/l/d***	Rat, prenatal male/female rat, 1. Generation, male/female rat 2. Generation, male/female***		EPA OPPTS 870.3800 Inhalation***	read across***
Developmental Toxicity	NOAEC: 3 mg/l/d***	rat		OECD 414, Inhalative	Maternal toxicity
Developmental Toxicity	NOAEC: 12 mg/l/d***	rat		OECD 414, Inhalative	Teratogenicity
Carcinogenicity***	NOAEC: >= 5,9 mg/l/d (103 weeks)***	rat mouse male/female***		OECD 451, Inhalative***	

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CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

Evaluation

In vitro tests did not show mutagenic effects

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Main symptoms

shortness of breath, abdominal pain, circulatory collapse, cough.

Target Organ Systemic Toxicant - Single exposure

Based on available data, the classification criteria are not met for:
STOT SE

Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:
STOT RE

Other adverse effects

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Components of the product may be absorbed into the body by inhalation and ingestion.

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:

<http://echa.europa.eu/information-on-chemicals/registered-substances>.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Isobutyraldehyde (78-84-2)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 277 mg/l	79/831/EEC.C2
Desmodesmus subspicatus	72h	EC50: 84 mg/l (Growth rate)	DIN 38412, part 9
Pimephales promelas (fathead minnow)	96h	LC50: 23 mg/l	
Pseudomonas putida	17 h	EC50: 468 mg/l	DIN 38412, part 8
Activated sludge (bacteriae)***	14 d***	NOEC: 100 mg/l***	OECD 301 C***

12.2. Persistence and degradability

Isobutyraldehyde, CAS: 78-84-2

Biodegradation

80 - 90 % (14 d), BOD, activated sludge, non-adapted, aerobic, OECD 301 C.***

Abiotic Degradation		
Isobutyraldehyde (78-84-2)		
Type	Result	Method
Hydrolysis***	No data available***	
Photolysis***	Half-life (DT50): 16,54 h***	calculated***

12.3. Bioaccumulative potential

Isobutyraldehyde (78-84-2)		
Type	Result	Method
log Pow	0,77 @ 25 °C (77 °F)***	OECD 107
BCF***	Significant bioaccumulation not to be expected***	

12.4. Mobility in soil

Isobutyraldehyde, CAS: 78-84-2

No data available

Isobutyraldehyde (78-84-2)		
Type	Result	Method
Surface tension***	Surface activity not expected***	
Adsorption/Desorption***	log Koc: 0,18 @ 25 °C***	
Distribution to environmental	Air: 90,5 % Soil: 0,0044 % Water:	Calculation according Mackay,

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compartments***	9,46 % Sediment: 0,00445 %***	Level I***
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12.5. Results of PBT and vPvB assessment

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PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

12.6. Other adverse effects

Isobutyraldehyde, CAS: 78-84-2

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Hazardous waste according to European Waste Catalogue (EWC)

Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

SECTION 14: Transport information

ICAO-TI / IATA-DGR

14.1. UN number	UN 2045
14.2. UN proper shipping name	Isobutyraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number	UN 2045
14.2. UN proper shipping name	Isobutyraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
EmS	F-E, S-D

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14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Product name	Butyraldehyde
Ship type	3
Pollution category	Y

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI
not listed

International Inventories

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AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2011496 (EU)
ENCS (2)-494 (JP)
ISHL (2)-494 (JP)
KECI 97-3-9 (KR)
KECI KE-24862 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)
TCSI (TW)

National regulatory information India

Hazardous Chemicals, Schedule 2: Threshold Quantities at an Isolated Storage
not listed

Hazardous Chemicals, Schedule 3: Threshold Quantities in an Industrial Installation
not listed

For details and further information please refer to the original regulation.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3

H225: Highly flammable liquid and vapour.

H319: Causes serious eye irritation.

Abbreviations

A table of terms and abbreviations can be found under the following link:

http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

Training advice

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For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet

Information contained in this safety data sheet is based on OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet

Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the OQ homepage (www.chemicals.oq.com).

The annex is not required because the substance is registered as an intermediate under REACH

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

End of Safety Data Sheet