

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision
Supersedes Version

6.01
6.00***

Revision Date
Issuing date

10-Feb-2021
10-Feb-2021

SECTION 1: Identification

1.1. Product identifier

Identification of the
substance/preparation

Isobutyraldehyde

CAS-No

78-84-2

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

Use of the Substance /
Preparation

Intermediate

Uses advised against

None

1.3. Details of the supplier of the safety data sheet

Supplier

OQ Chemicals Corporation
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA
Phone +1 346 378 7300

Product Information

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

1.4. Emergency telephone number

Emergency telephone number

NCEC +1 202 464 2554
available 24/7

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Serious eye damage/eye irritation Category 2A, H319

Flammable liquid Category 2, H225

Environmental hazard Aquatic Acute 3; H402

OSHA Specified Hazards

Not applicable.

Emergency telephone number
1 / 15

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SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

Hazard symbol(s)



Signal word

Danger

Hazard statements

H225: Highly flammable liquid and vapor.
H319: Causes serious eye irritation.
H402: Harmful to aquatic life

Precautionary statements

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.
P264: Wash hands thoroughly after handling.
P273: Avoid release to the environment.
P280: Wear protective gloves/eye protection/face protection.

Response

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.

Storage

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

Disposal

P501: Dispose of contents/container in accordance with local regulation.

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

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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

SECTION 3: Composition / information on ingredients

3.1. Substances

| Component | CAS-No | Concentration (%) |
|------------------|---------------|--------------------------|
| Isobutyraldehyde | 78-84-2 | > 97 |
| Water | 7732-18-5 | < 2,50 |

Remarks

Substance manufactured in Europe contains the following stabilizer(s): Triethanolamine.

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.

Skin

Wash off immediately with soap and plenty of water. 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.

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.

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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

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

Emergency telephone number
4 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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 spilled 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
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

Emergency telephone number
5 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

mild steel

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.

Note

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

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.

Individual protection measures, such as 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

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

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.

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 |

Skin and body protection

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

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision

6.01

Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (dust). Equipment should conform to NIOSH.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emission 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 | -86,62 °F (-65,9 °C) |
| Boiling point/range | 147,92 °F (64,4 °C) @ 1 atm (101,3 kPa) |
| Flash point | -9,4 °F (-23 °C) @ 1 atm (101,3 kPa) ^{***} |
| 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 |
|-----------------------|-------------------------------|--------------|------|------|--------|
| 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 @ 77 °F (25 °C), in water
0,77 @ 25 °C (77 °F) OECD 107^{***}

log Pow

Autoignition temperature

356 °F (180 °C) @ 1 atm (101,3 kPa)^{***}
Method
ASTM E 659

Decomposition temperature

No data available

Viscosity

0,43 mPa*s @ 68 °F (20 °C)
Method
ISO 3219, dynamic^{***}

9.2. Other information

Molecular weight

72,11

Molecular formula

C₄H₈O

Emergency telephone number
7 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

| | |
|-----------------------------|---|
| log Koc | 0,18 @ 25°C (77 °F) calculated*** |
| Oxidizing properties | Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties |
| Refractive Index | 1,373 @ 68 °F (20 °C) |
| Heat of combustion | 600 kcal/kg |
| Explosive properties | Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties |

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.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

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

Isobutyraldehyde, CAS: 78-84-2

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

Emergency telephone number
8 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision

6.01

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

| 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 |

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision

6.01

Isobutyraldehyde, CAS: 78-84-2

Assessment

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

Isobutyraldehyde, CAS: 78-84-2

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

Isobutyraldehyde, CAS: 78-84-2

Other adverse effects

Emergency telephone number
10 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

| Isobutyraldehyde (78-84-2) | | |
|---|---|--|
| Type | Result | Method |
| Surface tension*** | Surface activity not expected*** | |
| Adsorption/Desorption*** | log Koc: 0,18 @ 25 °C*** | |
| Distribution to environmental compartments*** | Air: 90,5 % Soil: 0,0044 % Water: 9,46 % Sediment: 0,00445 %*** | Calculation according Mackay, Level I*** |

12.5. Results of PBT and vPvB assessment

Isobutyraldehyde, CAS: 78-84-2

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.

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

D.O.T. (49CFR)

| | |
|------------------------------------|------------------|
| 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 | |
| Emergency Response Guide | 130 |

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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

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

Federal and State Regulations

Components of the product are listed in the quoted regulations. For details please refer to the regulations directly. This list is not exhaustive, please check for other applicable regulations.

Federal Regulations

This product is listed on the TSCA inventory

Section 313 Supplier Notification

This product contains the following toxic chemicals subject to the reporting requirements of Section 313 of the Emergency Planning and Community Right-To-Know Act of 1986 and of 40 CFR 372:

| Component | CAS-No | Concentration (%) |
|------------------|---------|-------------------|
| Isobutyraldehyde | 78-84-2 | > 97 |

This information must be included in all SDSs that are copied and distributed for this material.

Isobutyraldehyde, CAS: 78-84-2

Emergency telephone number
13 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision

6.01

EPCRA SARA Title III 313
de minimis concentration 1.0 %

State Regulations

Isobutyraldehyde, CAS: 78-84-2

MA RTK List
MN Hazardous Substances List
NJ RTK List
NY RTK List
PA RTK List

International Inventories

Isobutyraldehyde, CAS: 78-84-2

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)

SECTION 16: Other information

Revision Date 10-Feb-2021
Issuing date 10-Feb-2021

Hazard Rating Systems

NFPA (National Fire Protection Association)

Health Hazard 2
Fire Hazard 3
Reactivity 1

HMIS (Hazardous Material Information System)

Health Hazard 2
Flammability 3
Physical Hazard 1

Training advice

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

Emergency telephone number
14 / 15

NCEC +1 202 464 2554
USA (A-US)

SAFETY DATA SHEET



Isobutyraldehyde
10280

Version / Revision 6.01

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 use of a comma in section 3 and section 7 to 12 is the same as a period.

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End of Safety Data Sheet