

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description:	<u>Isobutyraldehyde</u>
Cat No. :	A12106
Synonyms	2-Methylpropanal; 2-Methylpropionaldehyde
CAS No	78-84-2
Molecular Formula	C4 H8 O
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Sector of use	SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category	PC21 - Laboratory chemicals
Process categories	PROC15 - Use as a laboratory reagent
Environmental release category	ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
Uses advised against	No Information available

1.3. Details of the supplier of the safety data sheet

Company	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
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E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Flammable liquids

Category 2 (H225)

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Health hazards

Serious Eye Damage/Eye Irritation

Category 2 (H319)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H225 - Highly flammable liquid and vapor

H319 - Causes serious eye irritation

Precautionary Statements

P240 - Ground and bond container and receiving equipment

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

Toxic to terrestrial vertebrates

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Isobutyraldehyde	78-84-2	EEC No. 201-149-6	<=100	Flam Liq. 2 (H225) Eye Irrit. 2 (H319)

REACH registration number

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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.
Ingestion	Do NOT induce vomiting. Get medical attention.
Inhalation	Remove to fresh air. Get medical attention immediately if symptoms occur. If not breathing, give artificial respiration.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician Treat symptomatically. Symptoms may be delayed.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

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6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information. Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. Ground/Bond container and receiving equipment. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Flammables area. Keep away from heat, sparks and flame. Keep container tightly closed in a dry and well-ventilated place. Keep refrigerated.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

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Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isobutyraldehyde 78-84-2 (<=100)			DNEL = 120mg/m ³	

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
Isobutyraldehyde 78-84-2 (<=100)	PNEC = 0.023mg/L	PNEC = 0.0863mg/kg sediment dw	PNEC = 0.23mg/L	PNEC = 10mg/L	PNEC = 0.00375mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Isobutyraldehyde 78-84-2 (<=100)	PNEC = 0.0023mg/L	PNEC = 0.00863mg/kg sediment dw			

8.2. Exposure controls

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Viton (R)	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Small scale/Laboratory use Maintain adequate ventilation

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Environmental exposure controls Prevent product from entering drains.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	-65 °C / -85 °F	
Softening Point	No data available	
Boiling Point/Range	63 °C / 145.4 °F	@ 760 mmHg
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Explosion limits Lower 1.6 Vol% Upper 10.6 Vol%	
Flash Point	-24 °C / -11.2 °F	Method - No information available
Autoignition Temperature	190 °C / 374 °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	0.45 mPa.s at 20 °C	
Water Solubility	75 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Isobutyraldehyde	0.77	
Vapor Pressure	189 mbar @ 20 °C	
Density / Specific Gravity	0.790	
Bulk Density	Not applicable	Liquid
Vapor Density	2.5 (Air = 1.0)	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C4 H8 O
Molecular Weight	72.11
Explosive Properties	Vapors may form explosive mixtures with air

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Air sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid Incompatible products. Excess heat. Keep away from open flames, hot surfaces and

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sources of ignition. Exposure to air.

10.5. Incompatible materials

Strong acids. Strong bases. Oxidizing agent.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

No acute toxicity information is available for this product

(a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isobutyraldehyde	3730 mg/kg (Rat)	LD50 = 5630 mg/kg (Rabbit)	LC50 > 23.6 mg/L (Rat) 4 h

(b) skin corrosion/irritation;

Based on available data, the classification criteria are not met

(c) serious eye damage/irritation;

Category 2

(d) respiratory or skin sensitization;

Respiratory

Based on available data, the classification criteria are not met

Skin

Based on available data, the classification criteria are not met

(e) germ cell mutagenicity;

Based on available data, the classification criteria are not met

Animal experiments showed mutagenic and teratogenic effects

(f) carcinogenicity;

Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

Based on available data, the classification criteria are not met

(h) STOT-single exposure;

Based on available data, the classification criteria are not met

(i) STOT-repeated exposure;

Based on available data, the classification criteria are not met

Target Organs

None known.

(j) aspiration hazard;

Based on available data, the classification criteria are not met

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

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11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

Do not empty into drains. Contains a substance which is: Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Isobutyraldehyde	LC50: 86 mg/L/48h (Leuciscus idus)	EC50: = 277 mg/L, 48h (Daphnia magna Straus)	EC50: = 84 mg/L, 72h (Desmodesmus subspicatus)

Component	Microtox	M-Factor
Isobutyraldehyde	EC50 = 468 mg/L 17 h	

12.2. Persistence and degradability

Persistence

Degradation in sewage treatment plant

Expected to be biodegradable
Persistence is unlikely, based on information available.
Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Isobutyraldehyde	0.77	No data available

12.4. Mobility in soil

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

12.5. Results of PBT and vPvB assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers

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retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN2045
14.2. UN proper shipping name ISOBUTYRALDEHYDE
14.3. Transport hazard class(es) 3
14.4. Packing group II

ADR

14.1. UN number UN2045
14.2. UN proper shipping name ISOBUTYRALDEHYDE
14.3. Transport hazard class(es) 3
14.4. Packing group II

IATA

14.1. UN number UN2045
14.2. UN proper shipping name ISOBUTYRALDEHYDE
14.3. Transport hazard class(es) 3
14.4. Packing group II

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Isobutyraldehyde	78-84-2	201-149-6	-	-	X	X	KE-24862	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
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Isobutyraldehyde	78-84-2	X	ACTIVE	X	-	X	X	X
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Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isobutyraldehyde	78-84-2	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Isobutyraldehyde	78-84-2	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Isobutyraldehyde	WGK1	

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H225 - Highly flammable liquid and vapor

H319 - Causes serious eye irritation

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Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Chemical incident response training.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

Prepared By

Health, Safety and Environmental Department

Creation Date

09-Jun-2010

Revision Date

09-Feb-2024

Revision Summary

New emergency telephone response service provider.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet