

Classified as hazardous in accordance with the criteria of EPA New Zealand

Section 1 - Identification

Product Identifier

Product Name	<u>3-Methylbutyraldehyde</u>
CAS No	590-86-3
Synonyms	Isovaleraldehyde
Molecular Formula	C5 H10 O
Molecular Weight	86.13
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

Product Code	163970000; 163970025; 163971000; 163975000
Address	Thermo Fisher Scientific New Zealand Ltd 244 Bush Road, Albany, Auckland, New Zealand
Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Telephone / Fax Numbers	Tel: 09 980 6700 Fax: 09 980 6788
E-mail address	ANZinfo@thermofisher.com

Section 2 - Hazard(s) Identification

Classification under Work Safe New Zealand

Classified as hazardous in accordance with the criteria of EPA New Zealand

HSNO Approval Number HSR002495

GHS Classification

Physical hazards

Flammable liquids

Category 2

Health hazards

Skin Corrosion/Irritation

Category 2

Serious Eye Damage/Eye Irritation

Category 2

Skin Sensitization

Category 1

Specific target organ toxicity - (single exposure)

Category 3

Environmental hazards

Chronic aquatic toxicity

Category 2

Label Elements**Signal Word****Danger****Hazard Statements**

H225 - Highly flammable liquid and vapor
H317 - May cause an allergic skin reaction
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H411 - Toxic to aquatic life with long lasting effects
H315 - Causes skin irritation

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
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P264 - Wash face, hands and any exposed skin thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P272 - Contaminated work clothing should not be allowed out of the workplace
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P273 - Avoid release to the environment

Response

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P312 - Call a POISON CENTER or doctor if you feel unwell
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
P362 + P364 - Take off contaminated clothing and wash it before reuse
P391 - Collect spillage

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Other hazards which do not result in classification

Stench

Section 3 - Composition and Information on Ingredients

Component	CAS No	Weight %
Isopentaldehyde	590-86-3	>95

Section 4 - First Aid Measures

Description of first aid measures

General Advice	If symptoms persist, call a physician.
New Zealand Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
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. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Self-Protection of the First Aider	Remove all sources of ignition. Use personal protective equipment as required.
First Aid Facilities	Eyewash, safety shower and washroom.
Most important symptoms and effects	None reasonably foreseeable. . May cause allergic skin reaction. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Notes to Physician	Treat symptomatically.

Section 5 - Fire Fighting Measures

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.

Specific Hazards Arising from the Chemical

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).

Special protective equipment and precautions for fire fighters

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

Personal Precautions, Protective Equipment and Emergency Procedures**Emergency procedures**

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

Environmental Precautions

Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean 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.

Precautions to prevent secondary hazards

Clean contaminated objects and areas thoroughly observing environmental regulations

Reference to Other Sections

Refer to protective measures listed in Sections 8 and 13.

Section 7 - Handling and Storage

Precautions for Safe Handling**Advice on safe handling**

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Hygiene Measures

When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

Conditions for Safe Storage, Including any Incompatibilities**Storage Conditions**

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

Incompatible Materials

Strong oxidizing agents. Strong bases. Strong reducing agents.

AS/NZS 2243.10:2004, Safety in laboratories - Storage of chemicals

AS 1940-2004 - The storage and handling of flammable and combustible liquids

Section 8 - Exposure Controls and Personal Protection

Control parameters**Exposure limits**

The product does not contain any hazardous materials with occupational exposure limits established.

Biological limit values

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

Appropriate engineering 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

Individual protection measures, such as personal protective equipment**Eye Protection**

Goggles (Australian/New Zealand Standard AS/NZS 1337 - Eye protectors for Industrial applications)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	AUS/NZ Standard	Glove comments
Nitrile rubber, Neoprene, Natural rubber, PVC.	See manufacturers recommendations	-	AS/NZS 2161	(minimum requirement)

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.

Skin and body protection Long sleeved clothing

Respiratory Protection Use an AS/NZS 1716 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained in line with AS/NZS 1715 on the use and maintenance of respiratory protective devices

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387 (or AUS/NZ equivalent)

Recommended half mask:- Valve filtering: EN405 or Half mask: EN140 plus filter, EN 141 (or AUS/NZ equivalent)
When RPE is used a face piece Fit Test should be conducted

Hygiene Measures When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

Environmental exposure controls Do not allow material to contaminate ground water system. Prevent product from entering drains.

Section 9 - Physical and Chemical Properties

Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless, Light yellow	
Odor	Stench	
Odor Threshold	No data available	
pH	5.3	
Melting Point/Range	-28 °C / -18.4 °F	
Softening Point	No data available	
Boiling Point/Range	91 - 93 °C / 195.8 - 199.4 °F	@ 760 mmHg
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 1.4 Vol% Upper 5.6 Vol%	
Flash Point	-5 °C / 23 °F	Method - No information available
Autoignition Temperature	235 °C / 455 °F	
Decomposition Temperature	No data available	
Viscosity	0.6 mPa s at 20 °C	
Water Solubility	Soluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Isopentaldehyde	1.5	
Vapor Pressure	57.9 mbar (20°C)	
Density / Specific Gravity	0.796	
Bulk Density	Not applicable	Liquid
Vapor Density	2.97 (Air = 1.0)	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

Other information

Molecular Formula	C5 H10 O
Molecular Weight	86.13
Explosive Properties	Vapors may form explosive mixtures with air

Section 10 - Stability and Reactivity

Reactivity	None known, based on information available
Stability	Air sensitive.
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.
Conditions to Avoid	Incompatible products, Excess heat, Keep away from open flames, hot surfaces and sources of ignition, Exposure to air.
Incompatible Materials	Strong oxidizing agents, Strong bases, Strong reducing agents.
Hazardous Decomposition Products	Carbon monoxide (CO). Carbon dioxide (CO ₂).

Section 11 - Toxicological Information

Acute Effects

Information on likely routes of exposure

Product Information

Inhalation	Irritating to respiratory system. May be harmful if inhaled.
Eyes	Irritating to eyes.
Skin	Irritating to skin. May be harmful in contact with skin.
Ingestion	May be harmful if swallowed. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea.

Numerical measures of toxicity

(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
Isopentaldehyde	LD50 = 5600 mg/kg (Rat)	LD50 = 2730 mg/kg (Rabbit)	LC50 = 42.7 mg/L (Rat) 4 h

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory	No data available
Skin	Category 1

Sensitization	May cause sensitization by skin contact
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
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. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

Section 12 - Ecological Information

Ecotoxicity

Aquatic ecotoxicity The product contains following substances which are hazardous for the environment. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Isopentaldehyde	LC50 96h 53 mg/L (Leuciscus idus)	EC50: = 177 mg/L, 48h (Daphnia magna)	EC50: = 78 mg/L, 96h (Desmodesmus subspicatus) EC50: = 80 mg/L, 72h (Desmodesmus subspicatus)	

Terrestrial ecotoxicity There is no data for this product

Persistence and Degradability Readily biodegradable

Persistence Soluble in water, Persistence is unlikely, based on information available.

Degradation in sewage treatment plant Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Isopentaldehyde	1.5	No data available

Mobility The product is water soluble, and may spread in water systems. . Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

Other adverse effects

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

Section 13 - Disposal Considerations

Waste treatment methods

Waste from Residues/Unused Products Do not allow into drains or watercourses or dispose of where ground or surface waters may be affected. Wastes, including emptied containers, are controlled wastes and should be disposed of in accordance with all federal, E.P.A., state and local regulations. Assure conformity with all applicable regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

Other Information Disposal agencies or waste contractors must comply with the New Zealand Hazardous Substances (Disposal) Regulations . 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. Do not let this chemical enter the environment. Do not empty into drains.

Section 14 - Transport Information

NZS 5433:2020

UN-No UN2058
Proper Shipping Name VALERALDEHYDE
Hazard Class 3
Packing Group II

IATA

UN-No UN2058
Proper Shipping Name VALERALDEHYDE
Hazard Class 3
Packing Group II

IMDG/IMO

UN-No UN2058
Proper Shipping Name VALERALDEHYDE
Hazard Class 3
Packing Group II

Environmental hazards Dangerous for the environment
Product is a marine pollutant according to the criteria set by IMDG/IMO

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable, packaged goods

Special Precautions No special precautions required. Please refer to the applicable dangerous goods regulations for additional information.

Additional information None known

Section 15 - Regulatory Information

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

HSNO Approval Number	HSR002495
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National Regulations

There are no applicable tolerable exposure limits or environmental exposure limits according to the EPA Controls for Hazardous Substances

Certified handlers, tracking and controlled substance license requirements

Certified handlers are required for some substances. This includes substances requiring a controlled substance license, and most explosives, vertebrates toxic agents, and certain fumigants. Acutely toxic substances which are a Category 1 or 2, such as pesticides also require Certified handlers. Please check the Health and Safety at Work Act 2015 for further information. Tracking is required for some highly hazardous substances. These substances need to be under the control of an appropriately trained person or appropriately secured. Please check the Health and Safety at Work Act 2015 for further information.

Prohibition or notification/licensing requirements

Shown below are details of specific prohibition/notifications or licensing requirements when they apply.

International Regulations

Ozone Depletion Potential This product does not contain any known or suspected substance

Persistent Organic Pollutant This product does not contain any known or suspected substance

Rotterdam Convention (PIC) Not applicable

Authorisation/Restrictions according to EU REACH Not applicable

International Inventories

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

Component	CAS No	NZIoC	AICS	EINECS	ELINCS	NLP	KECL	IECSC	TCSI
Isopentaldehyde	590-86-3	X	X	209-691-5	-	-	KE-23536	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	PICCS	ISHL	ENCS
Isopentaldehyde	590-86-3	X	ACTIVE	X	-	X	X	X

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Section 16 - Other Information

This safety data sheet complies with the requirements of the EPA Hazardous Substances (Hazard Classification) Notice 2020 and WorkSafe New Zealand Regulations

Legend

NZIoC - New Zealand Inventory of Chemicals	AICS - Australian Inventory of Chemical Substances
TSCA - United States Toxic Substances Control Act Section 8(b) Inventory	EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances
DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List	ENCS - Japanese Existing and New Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances	KECL - Korean Existing and Evaluated Chemical Substances
PICCS - Philippines Inventory of Chemicals and Chemical Substances	CAS - Chemical Abstracts Service
TWA - Time Weighted Average	ACGIH - American Conference of Governmental Industrial Hygienists
IARC - International Agency for Research on Cancer	PNEC - Predicted No Effect Concentration
NZS 5433:2020 - Transport of Dangerous Goods on Land	OECD - Organisation for Economic Co-operation and Development
ICAO/IATA - International Civil Aviation Organization/International Air Transport Association	IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
MARPOL - International Convention for the Prevention of Pollution from Ships	ADG - Australian Code for the Transport of Dangerous Goods by Road and Rail
LD50 - Lethal Dose 50%	LC50 - Lethal Concentration 50%
EC50 - Effective Concentration 50%	ATE - Acute Toxicity Estimate
WEL - Workplace Exposure Limit	RPE - Respiratory Protective Equipment
DNEL - Derived No Effect Level	NOEC - No Observed Effect Concentration
POW - Partition coefficient Octanol:Water	BCF - Bioconcentration factor
vPvB - very Persistent, very Bioaccumulative	PBT - Persistent, Bioaccumulative, Toxic
VOC - (Volatile Organic Compound)	

Key literature references and sources for data

HSNO classifications provided in the New Zealand Chemical Classification Information Database (CCID).

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

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

EPA Guide to classifying hazardous substances in New Zealand

EPA - Assigning a product to an existing HSNO approval guide

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.

Revision Date	10-Mar-2023
Revision Summary	Not applicable

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