

Isovaleraldehyde

sc-250204



The Power is Question

Material Safety Data Sheet

Hazard Alert Code Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

Isovaleraldehyde

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

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EMERGENCY

ChemWatch

Within the US & Canada: 877-715-9305

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(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS

C5-H10-O, (CH3)2CHCH2CHO, "butyraldehyde, 3-methyl-", "1-butanal, 3-methyl-", "isoamyl aldehyde", isopentaldehyde, isovaleral, "isovaleric aldehyde", 2-methylbutanal-4, 3-methylbutanal

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

	Min	Max
Flammability:	3	
Toxicity:	0	
Body Contact:	2	
Reactivity:	2	
Chronic:	2	

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

HARMFUL - May cause lung damage if swallowed.
Irritating to eyes, respiratory system and skin.
Highly flammable.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Swallowing of the liquid may cause aspiration into the lungs with the risk of chemical pneumonitis; serious consequences may result. (ICSC13733).

■ Although ingestion is not thought to produce harmful effects, the material may still be damaging to the health of the individual following ingestion, especially where pre-existing organ (e.

g.

EYE

■ There is some evidence that material may produce eye irritation in some persons and produce eye damage 24 hours or more after instillation.

Moderate inflammation may be expected with redness; conjunctivitis may occur with prolonged exposure.

SKIN

■ The material may cause mild but significant inflammation of the skin either following direct contact or after a delay of some time.

Repeated exposure can cause contact dermatitis which is characterized by redness, swelling and blistering.

■ Skin contact is not thought to have harmful health effects, however the material may still produce health damage following entry through wounds, lesions or abrasions.

■ Open cuts, abraded or irritated skin should not be exposed to this material.

■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ The material can cause respiratory irritation in some persons.

The body's response to such irritation can cause further lung damage.

■ Inhalation of vapours may cause drowsiness and dizziness.

This may be accompanied by narcosis, reduced alertness, loss of reflexes, lack of coordination and vertigo.

■ Exposure to aldehydes causes neurological symptoms such as headache, drowsiness, dizziness, seizures, depression and coma.

Cardiovascular involvement may result in increased heart rate, collapse and low blood pressure; respiratory effects include throat spasms, irritation, difficulty swallowing, pulmonary edema and an asthma-like condition.

CHRONIC HEALTH EFFECTS

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

There is limited evidence that, skin contact with this product is more likely to cause a sensitization reaction in some persons compared to the general population.

Exposure to Aliphatic aldehydes can cause irritation of the skin.

Chronic solvent inhalation exposures may result in nervous system impairment and liver and blood changes. [PATTYS].

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
iso-valeraldehyde	590-86-3	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

· Immediately give a glass of water. · First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor. · If spontaneous vomiting appears imminent or occurs, hold patient's head down, lower than their hips to help avoid possible aspiration of vomitus.

EYE

■ If this product comes in contact with the eyes: · Wash out immediately with fresh running water. · Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN

■ If skin contact occurs: · Immediately remove all contaminated clothing, including footwear · Flush skin and hair with running water (and soap if available).

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN

■ Any material aspirated during vomiting may produce lung injury. Therefore emesis should not be induced mechanically or pharmacologically.

Treat symptomatically.

for simple aldehydes.

-----BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.

Section 5 - FIRE FIGHTING MEASURES

Vapor Pressure (mmHg):	30.002 @ 20 C
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.803
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

- Alcohol stable foam.
- Dry chemical powder.

FIRE FIGHTING

- Alert Emergency Responders and tell them location and nature of hazard.
- May be violently or explosively reactive.

When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 1000 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Liquid and vapor are highly flammable.
- Severe fire hazard when exposed to heat, flame and/or oxidizers.

Combustion products include: carbon dioxide (CO₂), other pyrolysis products typical of burning organic material.

WARNING: Long standing in contact with air and light may result in the formation of potentially explosive peroxides.

FIRE INCOMPATIBILITY

- Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:

Chemical goggles.

Gloves:

Respirator:

Type A Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.

MAJOR SPILLS

- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Containers, even those that have been emptied, may contain explosive vapours.
- Do NOT cut, drill, grind, weld or perform similar operations on or near containers.
- DO NOT allow clothing wet with material to stay in contact with skin.
- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

- Packing as supplied by manufacturer. Plastic containers may only be used if approved for flammable liquid.

- For low viscosity materials (i): Drums and jerricans must be of the non-removable head type. (ii): Where a can is to be used as an inner package, the can must have a screwed enclosure.
- For materials with a viscosity of at least 2680 cSt. (23 deg. C).

STORAGE REQUIREMENTS

- Store in original containers in approved flame-proof area.
 - No smoking, naked lights, heat or ignition sources.
- Light and air sensitive.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

PERSONAL PROTECTION



RESPIRATOR

Type A Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE

- Safety glasses with side shields.
- Chemical goggles.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.

NOTE: The material may produce skin sensitization in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

· When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.

· When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.

· Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

OTHER

- Overalls.
- PVC Apron.
- Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity.
- For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets), non sparking safety footwear.

ENGINEERING CONTROLS

■ For flammable liquids and flammable gases, local exhaust ventilation or a process enclosure ventilation system may be required. Ventilation equipment should be explosion-resistant.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Mixes with water.

State	LIQUID	Molecular Weight	86.14
Melting Range (°F)	-59.8	Viscosity	Not Available
Boiling Range (°F)	194	Solubility in water (g/L)	Miscible
Flash Point (°F)	28.994	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	464	Vapor Pressure (mmHg)	30.002 @ 20 C
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	0.803
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	2.96
Volatile Component (%vol)	100	Evaporation Rate	Not available

APPEARANCE

Colourless liquid with apple-like odour; mixes with water (20 g/l). Soluble in alcohol and ether.

Isovaleraldehyde has a log Kow of 1.3, a water solubility of 20 g/l and a vapour pressure of 61 hPa. Based on the high vapour pressure of the substance isovaleraldehyde tends to pass from water to air. A measured log Kow of 1.31 indicates that there is no considerable potential for bio- or geoaccumulation.

Material	Value
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Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

STORAGE INCOMPATIBILITY

- Flammable and/or toxic gases are generated by the combination of aldehydes with azo, diazo compounds, dithiocarbamates, nitrides, and strong reducing agents.
 - Many aldehydes are incompatible with strong acids, amines, strong oxidizers, and alkaline materials.
- Avoid reaction with oxidizing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

iso-valeraldehyde

TOXICITY AND IRRITATION

ISO-VALERALDEHYDE:

- unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

TOXICITY	IRRITATION
Oral (rat) LD50: 5600 mg/kg	Skin (rabbit): 500 mg/24h - Mild
Inhalation (rat) LC50: 90860 mg/m ³	Eye (rabbit): 100 mg/24h - Moderate
Oral (mouse) LD50: 4750 mg/kg	
Inhalation (mouse) LC50: 50770 mg/m ³	
Dermal (rabbit) LD50: 3180 mg/kg	
Oral (guinea pig) LD50: 2950 mg/kg	

■ Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

for isovaleraldehyde: (syn: 3-methylbutyraldehyde)

Isovaleraldehyde is an irritating fluid of unpleasant odor, which at excessive doses may be absorbed into the body via all routes of exposure (oral, dermal and inhalation). Under practical conditions the irritation potential and chemical reactivity, however, would preclude significant systemic absorption.

Biotransformation occurs through the usual oxidative pathway, mediated by aldehyde dehydrogenase to isovaleric acid, which may be incorporated into the intermediary metabolism. Furthermore, isovaleric acid and- transiently- also isovaleraldehyde may arise from isovaleric alcohol (3-methylbutanol). For that reason, toxicity data from this alcohol and also from isovaleric acid may help in the assessment of potential systemic effects of isovaleraldehyde (i.e. this part of toxicity which is not mediated by the protein-reactive aldehyde function).

Isovaleraldehyde is low in general acute toxicity after oral, dermal or inhalation exposure, is clearly irritating to the eyes and is strongly irritant to the skin under occlusive conditions. The material is not regarded as a potent sensitiser which is a common experience for aliphatic aldehydes with a single aldehyde function in the molecule supported by the negative animal data from the structural analogous aldehydes n-butyraldehyde, n- valeraldehyde and 2-methylbutanal. Studies with repeated exposure in animals (subchronic toxicity) do not exist with isovaleraldehyde. However, the relatively uniform toxicity profiles of aldehydes allow an estimation of these endpoints on the basis of data and results, which have been obtained during the investigation of other structurally related aldehydes, such as propionaldehyde, n-butyraldehyde and isobutyraldehyde. For systemic effects in the tested aldehydes the NOAEL for oral uptake is 300 mg/kg in rats, with effects on blood at > 600 mg/kg bw (n-butyraldehyde). For inhalation, the NOAELs with respect to systemic toxicity are > 150 ppm. Effects observed were reduced food consumption in females rats at 750 ppm (propionaldehyde); no systemic effects were found up to the highest concentration of 2,000 ppm in rats (n-butyraldehyde). At 4,000 and 8,000 ppm body weight depression and mortality were observed in 13-week and 2 -year studies in rats (isobutyraldehyde). In the metabolic precursor (3 -methylbutanol-1) the only effects at the highest dose of 1,250 mg/kg (drinking water, rats) were blood effects. With respect to irritation, there is a clear dependency on molecule size, water solubility and log Kow, indicating a NOAEL for isovaleraldehyde of > 51 ppm; butyraldehydes show a distinct lower irritating potential than propionaldehyde.

Genotoxicity: The genotoxicity of isovaleraldehyde was investigated in-vitro with negative results in the Ames test and questionable results on SCE-rate in human lymphocytes. The substance did not show DNA-damaging activity in a Bacillus subtilis study (Rec -Assay). A mouse micronucleus test after intraperitoneal administration in doses up to 100 mg/kg body weight was clearly negative with respect to clastogenicity and impairment of chromosome distribution in the course of mitosis. Thus, there is no concern with respect to genotoxicity.

Carcinogenicity: At present, there is no concern for carcinogenic effects of isovaleraldehyde. The experiments with isobutyraldehyde indicate a LOAEL for non- neoplastic effects of 500 ppm with weak local effects in female rats.

Developmental toxicity: Prenatal toxicity investigations have been carried out with propionaldehyde in rats and isobutyraldehyde in rats and 3-methylbutanol-1 in rats and rabbits. In these studies no prenatal defects and no high systemic toxicity was observed; hence, also isovaleric acid is not expected to exert prenatal toxicity. Isovaleric acid is , furthermore, also physiologically formed during the catabolism of leucine.

The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.

CARCINOGEN

VPVB_(VERY~	US - Maine Chemicals of High Concern List	Carcinogen	CA Prop 65; IARC; NTP 11th ROC
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Section 12 - ECOLOGICAL INFORMATION

This material and its container must be disposed of as hazardous waste.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
iso-valeraldehyde	LOW		LOW	HIGH

GESAMP/EHS COMPOSITE LIST - GESAMP Hazard Profiles

Name / EHS TRN A1a A1b A1 A2 B1 B2 C1 C2 C3 D1 D2 D3 E1 E2 E3 Cas No / RTECS No _____
 _____ Isovalera 139 731 1 NI 1 R 3 NI 0 0 0 2 2 D 2 ldehyde / 0 CAS:590- 86- 3 /

Legend: EHS=EHS Number (EHS=GESAMP Working Group on the Evaluation of the Hazards of Harmful Substances Carried by Ships) NRT=Net Register Tonnage, A1a=Bioaccumulation log Pow, A1b=Bioaccumulation BCF, A1=Bioaccumulation, A2=Biodegradation, B1=Acuteaquatic toxicity LC/ECIC50 (mg/l), B2=Chronic aquatic toxicity NOEC (mg/l), C1=Acute mammalian oral toxicity LD50 (mg/kg), C2=Acute mammalian dermal toxicity LD50 (mg/kg), C3=Acute mammalian inhalation toxicity LC50 (mg/kg), D1=Skin irritation & corrosion, D2=Eye irritation& corrosion, D3=Long-term health effects, E1=Tainting, E2=Physical effects on wildlife & benthic habitats, E3=Interference with coastal amenities, For column A2: R=Readily biodegradable, NR=Not readily biodegradable. For column D3: C=Carcinogen, M=Mutagenic, R=Reprotoxic, S=Sensitising, A=Aspiration hazard, T=Target organ systemic toxicity, L=Lunginjury, N=Neurotoxic, I=Immunotoxic. For column E1: NT=Not tainting (tested), T=Tainting test positive. For column E2: Fp=Persistent floater, F=Floater, S=Sinking substances. The numerical scales start from 0 (no hazard), while higher numbers reflect increasing hazard. (GESAMP/EHS Composite List of Hazard Profiles - Hazard evaluation of substances transported by ships)

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information

Ignitability characteristic: use EPA hazardous waste number D001 (waste code I)

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

! Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible.
- Consult manufacturer for recycling options or consult Waste Management Authority for disposal if no suitable treatment or disposal facility can be identified.

Section 14 - TRANSPORTATION INFORMATION

DOT:

Symbols: None Hazard class or Division: 3

Identification Numbers: UN2058 PG: II

Label Codes: 3 Special provisions: IB2, T4,

TP1

Packaging: Exceptions: 150 Packaging: Non- bulk: 202

Packaging: Exceptions: 150 Quantity limitations: 5 L

Passenger aircraft/rail:

Quantity Limitations: Cargo 60 L Vessel stowage: Location: B

aircraft only:

Vessel stowage: Other: None

Hazardous materials descriptions and proper shipping names:

Valeraldehyde

Air Transport IATA:

ICAO/IATA Class: 3 ICAO/IATA Subrisk: None
UN/ID Number: 2058 Packing Group: II
Special provisions: None
Cargo Only
Packing Instructions: 60 L Maximum Qty/Pack: 5 L
Passenger and Cargo Passenger and Cargo
Packing Instructions: 307 Maximum Qty/Pack: 305
Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity
Packing Instructions: 1 L Maximum Qty/Pack: Y305
Shipping Name: VALERALDEHYDE
Maritime Transport IMDG:
IMDG Class: 3 IMDG Subrisk: None
UN Number: 2058 Packing Group: II
EMS Number: F-E , S-D Special provisions: None
Limited Quantities: 1 L
Shipping Name: VALERALDEHYDE

Section 15 - REGULATORY INFORMATION

iso-valeraldehyde (CAS: 590-86-3) is found on the following regulatory lists;

"GESAMP/EHS Composite List - GESAMP Hazard Profiles", "IMO MARPOL 73/78 (Annex II) - List of Noxious Liquid Substances Carried in Bulk", "International Fragrance Association (IFRA) Survey: Transparency List", "OECD Representative List of High Production Volume (HPV) Chemicals", "US - Pennsylvania - Hazardous Substance List", "US EPA Master Testing List - Index I Chemicals Listed", "US Food Additive Database", "US -Texas Air Monitoring Comparison Values for Evaluating VOCs", "US Toxic Substances Control Act (TSCA) - Inventory", "US TSCA Section 8 (a) - Preliminary Assessment Information Rules (PAIR) - Reporting List", "US TSCA Section 8 (d) - Health and Safety Data Reporting"

Section 16 - OTHER INFORMATION

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■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.
A list of reference resources used to assist the committee may be found at:
www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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