SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.1
Creation Date: July 15, 2019
Revision Date: May 15, 2024

SECTION 1: Identification

1.1 GHS Product identifier

Product name Isovaleraldehyde

1.2 Other means of identification

Product number 590-86-3
Other names Butanal, 3-methyl-; ISOAMYLALDEHYDE; FEMA 2692

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.
Uses advised against no data available

1.4 Supplier's details

Company Zhongshan Greenrock Technology Co., Ltd.
Address Jinsan Avenue, Sanjiao Town, Zhongshan City, Guangdong Province, China
Telephone +86-2087066781

1.5 Emergency phone number

Emergency phone number +86-2087066781
Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 2
Skin sensitization, Category 1
Eye irritation, Category 2
Specific target organ toxicity – single exposure, Category 3
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

2.2 GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger
Hazard statement(s) H225 Highly flammable liquid and vapour
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

Precautionary statement(s)

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. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P272 Contaminated work clothing should not be allowed out of the workplace. P264 Wash ... thoroughly after handling. P271 Use only outdoors or in a well-ventilated area. P273 Avoid release to the environment.
Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower]. P370+P378 In case of fire: Use ... to extinguish. P302+P352 IF ON SKIN: Wash with plenty of water/... P333+P317 If skin irritation or rash occurs: Get medical help. P321 Specific treatment (see ... on this label). P362+P364 Take off contaminated clothing and wash it before reuse. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P319 Get medical help if you feel unwell. P391 Collect spillage.
Storage	P403+P235 Store in a well-ventilated place. Keep cool. P403+P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up.
Disposal	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Isovaleraldehyde	Isovaleraldehyde	590-86-3	209-691-5	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Rinse and then wash skin with water and soap.

Following eye contact

Rinse with plenty of water (remove contact lenses if easily possible).

Following ingestion

Rinse mouth. Do NOT induce vomiting.

4.2 Most important symptoms/effects, acute and delayed

Inhalation causes chest discomfort, nausea, vomiting, and headache. Contact of liquid with eyes or skin causes irritation. Ingestion causes irritation of mouth and stomach. (USCG, 1999)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aldehydes and Related Compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Use "alcohol" foam, dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

5.3 Special protective actions for fire-fighters

Use dry sand, carbon dioxide, dry powder. NO water. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Remove all ignition sources. Evacuate danger area! Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

6.2 Environmental precautions

Remove all ignition sources. Evacuate danger area! Consult an expert! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or handling. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Well closed. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing.Materials which are toxic as stored or which can decompose into toxic components...should be stored in a cool, well ventilated place, out of the direct rays of the sun, away from areas of high fire hazard, and should be periodically inspected. Incompatible materials should be isolated...

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Component	Isovaleraldehyde			
CAS No.	590-86-3			
	Limit value - Eight hours		**Limit value - Short term**	
	ppm	**mg/m^3**	**ppm**	**mg/m^3**
Austria	10	39	10	39
Germany (AGS)	10	39	10 (1)	39 (1)
	Remarks			
Germany (AGS)	(1) 15 minutes average value			

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation. Avoid inhalation of mist.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid.
Colour	Colourless, clear.
Odour	Apple-like odor
Melting point/freezing point	< -90 °C.
Boiling point or initial boiling point and boiling range	92 °C. Atm. press.:1 013 hPa.
Flammability	Highly flammable.
Lower and upper explosion limit/flammability limit	Lower flammable limit: 1.7% by volume; Upper flammable limit: 6.8% by volume
Flash point	0.5 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature	210 °C. Atm. press.:1 020 hPa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	kinematic viscosity (in mm^2/s) = 0.69. Temperature:20°C. Remarks:The determination of the kinematic viscosity was carried out by the capillary method with a viscosimeter according to Ubbelohde.
Solubility	Miscible with water
Partition coefficient n-octanol/water	Pow = 31.5. Temperature:25 °C.;log Pow = 1.5. Temperature:25 °C.
Vapour pressure	75 hPa. Temperature:20 °C.
Density and/or relative density	796.9 kg/m^3. Temperature:20 °C.
Relative vapour density	2.96 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Decomposes on heating. This produces irritating fumes.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

The vapour is heavier than air and may travel along the ground; distant ignition possible. The vapour mixes well with air, explosive mixtures are easily formed.ISOVALERALDEHYDE is an aldehyde. Aldehydes are frequently involved in self-condensation or polymerization reactions. These reactions are exothermic; they are often catalyzed by acid. Aldehydes are readily oxidized to give carboxylic acids. Flammable and/or toxic gases are generated by the combination of aldehydes with azo, diazo compounds, dithiocarbamates, nitrides, and strong reducing agents. Aldehydes can react with air to give first peroxo acids, and ultimately carboxylic acids. These autoxidation reactions are activated by light, catalyzed by salts of transition metals, and are autocatalytic (catalyzed by the products of the reaction). The addition of stabilizers (antioxidants) to shipments of aldehydes retards autoxidation.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

Disaster hazard: slight; when heated, it emits acrid fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - ca. 5 740 mg/kg bw. Remarks:LD50 converted from the originally reported value of 7.2 mL/kg bw (based on a density of 0.797 g/cm^3.

- Inhalation: LC50 - rat - 42.7 mg/L air (nominal).
- Dermal: LD50 - rabbit (male) - 2 534 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes and respiratory tract. The substance is mildly irritating to the skin. If swallowed the substance may cause vomiting and could result in aspiration pneumonitis.

STOT-repeated exposure

no data available

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - Pimephales promelas - 3.25 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 177 mg/L - 48 h.
- Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 112.78 mg/L - 72 h.
- Toxicity to microorganisms: EC10 - Pseudomonas putida - 310 mg/L - 17 h.

12.2 Persistence and degradability

AEROBIC: In activated sludge from waste treatment plants, 3-methylbutanal had a theoretical oxygen demand of 9.2, 14.2, and 16.1% after 6, 12, and 24 hours, respectively(1).

12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for 3-methylbutanal(SRC), using a water solubility of 1.4X10+4 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

The Koc of 3-methylbutanal is estimated as 23(SRC), using a water solubility of 1.4X10+4 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 3-methylbutanal is expected to have very high mobility in soil.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN2058 (For reference only, please check.) IMDG: UN2058 (For reference only, please check.) IATA: UN2058 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: VALERALDEHYDE (For reference only, please check.) IMDG: VALERALDEHYDE (For reference only, please check.) IATA: VALERALDEHYDE (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.) IMDG: 3 (For reference only, please check.) IATA: 3 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: II (For reference only, please check.) IMDG: II (For reference only, please check.) IATA: II (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes IMDG: Yes IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Isovaleraldehyde	Isovaleraldehyde	590-86-3	209-691-5
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

Creation Date	July 15, 2019
Revision Date	May 15, 2024

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

Health effects of exposure to the substance have not been investigated adequately.

Any questions regarding this SDS, Please send your inquiry to export@greenrockchem.com

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