# SAFETY DATA SHEETS

According to Globally Harmonized System of Classification and Labelling of Chemicals (GHS) - Sixth revised edition

Version: 1.0

Creation Date: Aug 12, 2017

Revision Date: Aug 12, 2017

## 1. Identification

### 1.1 GHS Product identifier

| | |
|---|---|
| Product name | 3-methylbutanal |

### 1.2 Other means of identification

| | |
|---|---|
| Product number | - |
| Other names | Butanal, 3-methyl- |

### 1.3 Recommended use of the chemical and restrictions on use

| | |
|---|---|
| Identified uses | For industry use only. Food additives -> Flavoring Agents |
| Uses advised against | no data available |

## 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.

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 skin with water [or shower]. |
| | P370+P378 In case of fire: Use ... to extinguish. |
| | P302+P352 IF ON SKIN: Wash with plenty of water/... |
| | P333+P313 If skin irritation or rash occurs: Get medical advice/attention. |
| | 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. |
| | P337+P313 If eye irritation persists: Get medical advice/attention. |
| | P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. |
| | P312 Call a POISON CENTER/doctor/…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 ... |

## 2.3 Other hazards which do not result in classification

none

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# 3. Composition/information on ingredients

## 3.1 Substances

| Chemical name | Common names and synonyms | CAS number | EC number | Concentration |
|---|---|---|---|---|
| 3-methylbutanal | 3-methylbutanal | 590-86-3 | none | 100% |

# 4. First-aid measures

## 4.1 Description of necessary first-aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

Fresh air, rest.

In case of skin contact

Rinse and then wash skin with water and soap.

In case of eye contact

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

If swallowed

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

/SRP:/ 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/

## 5. Fire-fighting measures

### 5.1 Extinguishing media

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

Wear self-contained breathing apparatus for firefighting if necessary.

## 6. Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

### 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

Pick up and arrange disposal. Sweep up and shovel. Keep in suitable, closed containers for disposal.

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## 7. Handling and storage

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Avoid exposure - obtain special instructions before use.Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

### 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...

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## 8. Exposure controls/personal protection

### 8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

### 8.2 Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### 8.3 Individual protection measures, such as personal protective

equipment (PPE)

Eye/face protection

Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Wear impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace. Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique(without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

Wear dust mask when handling large quantities.

Thermal hazards

no data available

## 9. Physical and chemical properties

| | |
|---|---|
| Physical state | clear, colorless liquid. |
| Colour | Colorless liquid |
| Odour | Apple-like odor |
| Melting point/ freezing point | 283°C(lit.) |
| Boiling point or initial boiling point and boiling range | 300°C(lit.) |
| 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 | 3°C(lit.) |
| Auto-ignition temperature | 464 deg F (240°C) |
| Decomposition | no data available |

| | |
|---|---|
| temperature | |
| pH | no data available |
| Kinematic viscosity | 0.58 mPa.S at 20°C |
| Solubility | In water:15 g/L (20 °C) |
| Partition coefficient n-octanol/water (log value) | log Kow = 1.23 (est) |
| Vapour pressure | 30 mm Hg ( 20 °C) |
| Density and/or relative density | 0.796 |
| Relative vapour density | 2.96 (vs air) |
| Particle characteristics | no data available |

## 10. Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 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.

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# 11. Toxicological information

Acute toxicity

- Oral: LD50 Mouse oral 4750 mg/kg
- Inhalation: LC50 mouse inhalation approximately 6.2 mg/L/10 hrs.
- Dermal: no data available

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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

## 12. Ecological information

### 12.1 Toxicity

- Toxicity to fish: LC50; Species: Pimephales promelas (Fathead minnow, age 30 days, mean length 20.4 mm, mean weight 0.127 g); Conditions: flow through, 23.9°C pH 7.58, hardness 49.3 mg/L CaCO3, alkalinity 47.8 mg/L CaCO3, dissolved oxygen 6.9 mg/L; Concentration: 3.25 mg/L for 96 hr (95% confidence limit: 2.98-3.54 mg/L) /97.3% purity
- Toxicity to daphnia and other aquatic invertebrates: EC50; Species Daphnia magna (Water flea); Concentration: 210.0 mg/L for 24 hr; Effect: immobilization /Conditions of bioassay not specified in source examined
- Toxicity to algae: EC50; Species Scenedesmus subspicatus (Algae); Concentration: 80.0 mg/L for 72 hr; Effect: growth inhibition /Conditions of bioassay not specified in source examined
- Toxicity to microorganisms: no data available

### 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

## 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.

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# 14. Transport information

## 14.1 UN Number

ADR/RID: UN2058 IMDG: UN2058 IATA: UN2058

## 14.2 UN Proper Shipping Name

ADR/RID: VALERALDEHYDE
IMDG: VALERALDEHYDE
IATA: VALERALDEHYDE

## 14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

## 14.4 Packing group, if applicable

ADR/RID: II IMDG: II IATA: II

## 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 Annex II of MARPOL 73/78 and the IBC Code

no data available

## 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 |
|---|---|---|---|
| 3-methylbutanal | 3-methylbutanal | 590-86-3 | none |
| 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 | | | Not Listed. |
| Chinese Chemical Inventory of Existing Chemical Substances (China IECSC) | | | Listed. |

## 16. Other information

Information on revision

| | |
|---|---|
| Creation Date | Aug 12, 2017 |
| Revision Date | Aug 12, 2017 |

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/


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