

Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 02 Jun 2023

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product name:

3-Methylbutyraldehyde

1.1. Catalog No.:

688074

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

HPC Standards GmbH
Am Wieseneck 7

04451 Cunnersdorf
Deutschland

Tel. +49 34291 3372-36
Fax. +49 34291 3372-39
contact@hpc-standards.com

1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36
This number is only available during office hours.

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
Flammable liquids (Category 2), H225
Eye irritation (Category 2), H319
Skin sensitisation (Category 1), H317
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Long-term (chronic) aquatic hazard (Category 2), H411

2.2. Label elements

2.2.1. Pictogram



2.2.2.

2.2 Label elements
Labelling according Regulation (EC) No 1272/2008

Pictogram 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)

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

P273 Avoid release to the environment.

P280 Wear protective gloves.

P302 + P352 IF ON SKIN: Wash with plenty of water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard

Statements

none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : 3-Methylbutanal

NSC 404119

Formula : C₅H₁₀O

Molecular weight : 86,13 g/mol

CAS-No. : 590-86-3

EC-No. : 209-691-5

Component Classification Concentration

Isovaleraldehyde

Flam. Liq. 2; Eye Irrit. 2;

Skin Sens. 1; STOT SE 3;

Aquatic Chronic 2; H225,

H319, H317, H335, H411

<= 100 %

3.1.1. Formula

C₅H₁₀O

3.1.2. Molecular Weight (g/mol)

86.13

3.1.3. CAS-No.

590-86-3

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

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

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse

mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas.

Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand,

earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). 6.4 Reference to other sections
For disposal see section 13

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are

opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Recommended storage temperature 2 - 8 °C

Handle and store under inert gas. Air and light sensitive.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid

Colour: colourless

b) Odour unpleasant

c) Odour Threshold No data available

d) pH No data available

e) Melting

point/freezing point

Freezing point: < -90 °C

f) Initial boiling point

and boiling range

91 - 93 °C at 1013 hPa

g) Flash point 0,5 °C - closed cup

h) Evaporation rate No data available

i) Flammability (solid,
gas)

No data available

j) Upper/lower

flammability or

explosive limits

No data available

k) Vapour pressure 40 hPa at 20 °C

l) Vapour density 2,97 - (Air = 1.0)

m) Relative density 0,797 g/cm³

n) Water solubility 15 g/l at 20 °C - OECD Test Guideline 105 - soluble

o) Partition coefficient: log Pow: 1,5 at 25 °C n-octanol/water

p) Auto-ignition
temperature

210 °C

at 1.020 hPa

q) Decomposition
temperature

No data available

r) Viscosity 0,69 mm²/s at 20 °C -

s) Explosive properties No data available

t) Oxidizing properties No data available

9.2 Other safety information

Relative vapour
density

2,97 - (Air = 1.0)

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

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Oxidizing agents, Strong bases, Strong reducing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 5.600 mg/kg

Remarks: Behavioral: Somnolence (general depressed activity).

LD50 Oral - Rat - 5.740 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 42.700 mg/m³

Remarks: Behavioral: Altered sleep time (including change in righting reflex).

Gastrointestinal: Changes in structure or function of salivary glands.

LD50 Dermal - Rabbit - 2.534 mg/kg

Remarks: Liver: Other changes. Prolonged skin contact may cause skin irritation and/or dermatitis.

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 24 h Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes. - 8 d

Respiratory or skin sensitisation

The preceding data, or interpretation of data, was determined using Quantitative Structure
Activity Relationship (QSAR) modeling.

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is
identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: ES3450000

Nausea, Headache, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 3,25 mg/l - 96 h

Toxicity to daphnia

and other aquatic

invertebrates

EC50 - Daphnia magna (Water flea) - 177 mg/l - 48 h

Toxicity to algae ErC50 - Desmodesmus subspicatus (green algae) - 113 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability Result: 50 % - Not readily biodegradable.

(OECD Test Guideline 301D)

12.3 Bioaccumulative potential

Does not bioaccumulate.

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher

12.6 Other adverse effects

Toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: 1989 IMDG: 1989 IATA: 1989
14.2 UN proper shipping name
ADR/RID: ALDEHYDES, N.O.S. (Isovaleraldehyde)
IMDG: ALDEHYDES, N.O.S. (Isovaleraldehyde)
IATA: Aldehydes, n.o.s. (Isovaleraldehyde)
14.3 Transport hazard class(es)
ADR/RID: 3 IMDG: 3 IATA: 3
14.4 Packaging group
ADR/RID: II IMDG: II IATA: II
14.5 Environmental hazards
ADR/RID: no IMDG Marine pollutant: no IATA: no
14.6 Special precautions for user
No data available

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.
REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, preparations and articles (Annex XVII)
REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, preparations and articles (Annex XVII) 15.2 Chemical safety assessment
For this product a chemical safety assessment was not carried out

16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. For lab use only!