SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Isovaleric acid
Product Number : W310212
Brand : Aldrich
CAS-No. : 503-74-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word Danger
Hazard statement(s)
H227  Combustible liquid.
H314  Causes severe skin burns and eye damage.
H402  Harmful to aquatic life.

Precautionary statement(s)
P210  Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P264  Wash skin thoroughly after handling.
P273  Avoid release to the environment.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363  Wash contaminated clothing before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235 Store in a well-ventilated place. Keep cool.
P405  Store locked up.
P501  Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients
3.1 Substances
Synonyms : 3-Methylbutanoic acid
            3-Methylbutyric acid

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-methylbutyric acid</td>
<td>Flam. Liq. 4; Skin Corr. 1B; Eye Dam. 1; Aquatic Acute 3; H227, H314, H318, H402</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

In case of eye contact
After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Carbon dioxide (CO2) Foam Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
SECTION 6: Accidental release measures

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent and neutralising material (e.g. Chemizorb® H⁺, Merck Art. No. 101595). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

SECTION 7: Handling and storage

7.1 **Precautions for safe handling**

**Advice on protection against fire and explosion**
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage class**
Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

7.3 **Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 **Control parameters**

**Ingredients with workplace control parameters**
Contains no substances with occupational exposure limit values.
8.2 Exposure controls

**Appropriate engineering controls**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

**Skin protection**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

**Full contact**
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

**Splash contact**
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 240 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

**Body Protection**
protective clothing

**Respiratory protection**
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: liquid
   Color: colorless

b) Odor
   unpleasant

c) Odor Threshold
   No data available

d) pH
   3.1 at 10 g/l at 25 °C (77 °F) - DIN 19268

e) Melting point/freezing point
   Melting point: ca.-31 °C (ca.-24 °F) - OECD Test Guideline 102

f) Initial boiling point and boiling range
   178.5 °C 353.3 °F at 1,013 hPa - OECD Test Guideline 103

g) Flash point
   80 °C (176 °F) - Pensky-Martens closed cup - ISO 2719

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   Upper explosion limit: 6.8 %(V)
   Lower explosion limit: 1.5 %(V)

k) Vapor pressure
   ca.1 hPa at 20 °C (68 °F)

l) Vapor density
   No data available

m) Density
   0.93 g/cm3 at 20 °C (68 °F) - OECD Test Guideline 109
   Relative density
   No data available

n) Water solubility
   48 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - completely soluble

o) Partition coefficient: n-octanol/water
   Pow: 50; log Pow: 1.7 at 25 °C (77 °F) - Bioaccumulation is not expected.

p) Autoignition temperature
   420 °C (788 °F) at 988 hPa - Tested according to Directive 92/69/EEC.

q) Decomposition temperature
   > 300 °C (> 572 °F) -

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information

Surface tension
   63.3 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115

Dissociation constant
   4.7 at 20.1 °C (68.2 °F) - OECD Test Guideline 112
SECTION 10: Stability and reactivity

10.1 Reactivity
Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
Violent reactions possible with:
alkalines
Amines
Nitriles
Oxidizing agents

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
various metals

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 2,500 mg/kg
(OECD Test Guideline 401)
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Inhalation: Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Inhalation: Corrosive to respiratory system.
Dermal: No data available
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Corrosive - 3 min - 1 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Remarks: Causes serious eye damage.

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: Micronucleus test  
Species: Mouse  
Cell type: Red blood cells (erythrocytes)  
Application Route: Oral  
Method: OECD Test Guideline 474  
Result: negative  
Remarks: (in analogy to similar products)

**Carcinogenicity**

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

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

Repeated dose toxicity - Rat - male - Oral - 90 Days - NOAEL (No observed adverse effect level) - 5,000 mg/kg  
Remarks: (in analogy to similar products)  
(ECHA)  
The value is given in analogy to the following substances: Sodium isovalerate-1-13C

RTECS: NY1400000  
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Inhalation may provoke the following symptoms:; spasm, inflammation and edema of the bronchi, spasm, inflammation and edema of the larynx, pneumonitis, pulmonary edema, Symptoms and signs of poisoning are; burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Aldrich - W310212
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

Toxicity to fish static test LC50 - Pimephales promelas (fathead minnow) - 77 mg/l - 96 h (OECD Test Guideline 203)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: valeric acid

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 51.25 mg/l - 48 h (OECD Test Guideline 202)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: 2-methylpropionic acid; isobutyric acid

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata - 29.3 mg/l - 72 h (OECD Test Guideline 201)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: valeric acid

Static test NOEC - Pseudokirchneriella subcapitata - 6.38 mg/l - 72 h (OECD Test Guideline 201)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: valeric acid

Toxicity to bacteria fermentation tube test EC0 - activated sludge - > 1,000 mg/l
Remarks: (External MSDS)

12.2 Persistence and degradability
Biodegradability aerobic - Exposure time 10 d
Result: 58 - 66 % - Readily biodegradable.
(OECD Test Guideline 301C)

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
Discharge into the environment must be avoided.
SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 3265  Class: 8  Packing group: II
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 3265  Class: 8  Packing group: II  EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-methylbutyric acid)

IATA
UN number: 3265  Class: 8  Packing group: II
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-methylbutyric acid</td>
<td>503-74-2</td>
<td>1993-04-24</td>
</tr>
</tbody>
</table>

SECTION 16: Other information

Further 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
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.