

3-Methylbutanoic acid SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: 3-Methylbutanoic acid

* Catalog Number: S6287

* CAS Number: 503-74-2

* IUPAC Name: Butanoic acid, 3-methyl-

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals

* TollFree: +1 877 796-6397

* Tel: +1 832 582-8158

* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Skin corrosion: Category 1. H314

Serious eye damage: Category 1. H318

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H314: Causes severe skin burns and eye damage

H318: Causes serious eye damage

Precautionary statement(s)

None.

Prevention

P260: Do not breathe dust/fume/gas/mist/vapors/spray.

P264: Wash hands thoroughly after handling.

P264+P265: Wash hands thoroughly after handling. Do not touch eyes.

P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Response	<p>P301+P330: IF SWALLOWED: Rinse mouth.</p> <p>P302+P361: IF ON SKIN: Take off immediately all contaminated clothing.</p> <p>P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.</p> <p>P305+P354: IF IN EYES: Immediately rinse with water for several minutes.</p> <p>P316: Get emergency medical help immediately.</p> <p>P317: Get emergency medical help.</p> <p>P321: Specific treatment (see information on this label and safety datasheet)).</p> <p>P331: Do NOT induce vomiting.</p> <p>P338: Remove contact lenses, if present and easy to do. Continue rinsing.</p> <p>P354: Immediately rinse with water for several minutes.</p> <p>P363: Wash contaminated clothing before reuse.</p>
Storage	P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: 3-Methylbutanoic acid
 CAS Number: 503-74-2
 PubChem CID: 10430
 Molecular formula: C₅H₁₀O₂
 Molecular weight: 102.13 g/mol
 IUPAC name: 3-methylbutanoic acid

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

SMALL FIRE: Dry chemical, CO₂ or water spray.

LARGE FIRE: Dry chemical, CO₂, alcohol-resistant foam or water spray. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 70 °C

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with

environmental regulatory agencies for guidance on acceptable disposal practices.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. DO NOT GET WATER INSIDE CONTAINERS. (ERG, 2024)
KEEP TIGHTLY CLOSED.

7.2 Conditions for safe storage, including any incompatibilities

KEEP TIGHTLY CLOSED.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

Store in original container. Keep upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles and face shield.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: Isopentanoic acid is a colorless liquid with a penetrating odor. It is slightly soluble in water. It is corrosive to metals and to tissue.
- b) Odor: DISAGREEABLE, RANCID-CHEESE ODOR
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: -29.3 °C
- f) Initial boiling point and boiling range: 176.5 °C @ 760 MM HG
- g) Flash point: 70 °C
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: 0.44 [mmHg]
- l) Vapor density: No data available
- m) Relative density: 0.931 @ 20 °C/4 °C
- n) Water solubility: SOL IN 24 PARTS WATER; SOL IN ALCOHOL, ETHER, CHLOROFORM
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 1.2
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 37.3 Å²
Complexity: 66

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

Causes severe skin burns and eye damage (H314).

Serious eye damage/eye irritation:

Causes serious eye damage (H318).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

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

No additional toxicological information available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 Cyprinus carpio 2.1 mg/L/48 hr /Conditions of bioassay not specified/

Isovaleric acid occurs naturally in hop oil, tobacco and several other plants. Isovaleric acid's production and use in medicine, flavors, perfumes, as a chemical intermediate in fungicides, rodenticides, sedatives, narcotics, and other drugs may result in its release to the environment through various waste streams. If released to the atmosphere, isovaleric acid is expected to exist solely in the vapor phase in the ambient atmosphere based on a measured vapor pressure of 0.44 mm Hg at 25 °C. Vapor-phase isovaleric acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 3.9 days. If released to soil, an estimated Koc of 100 indicates that isovaleric acid is expected to have high mobility in soil. Isovaleric acid is not expected to volatilize from dry soil surfaces based on its vapor pressure. Volatilization from moist soil surfaces may occur based on a measured Henry's Law constant of 8.33×10^{-7} atm-cu m/mole at 25 °C. Isovaleric acid has the potential to biodegrade in both soil and water based upon results in aerobic aqueous screening tests and anaerobic die-away studies with ground water samples. If released into water, isovaleric acid is not expected to adsorb to suspended solids and sediment in the water column based on an estimated Koc of 100. The potential for bioconcentration in aquatic organism

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 1.2

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations.

Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

DOT label: Poison

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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:

Acute (short-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: Butanoic acid, 3-methyl-
- EFSA Legal Basis: Regulation (EC) No 1831/2003 (amended)
- New Jersey Worker and Community Right to Know Act: The New Jersey Worker and Community Right to Know Act requires public and private employers to provide information about hazardous substances at their workplaces. (N.J.S.A. 34:5A-1 et. seq.)
- FDA Requirements: Isovaleric acid is a food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant in accordance with the following conditions: 1) the quantity added to food does not exceed the amount reasonably required to accomplish its intended physical

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or

contact with the product.