ISOVALERIC ACID (1-13C, 99%)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 07/12/2015 Revision date: 28/07/2022 Supersedes: 07/12/2015 Version: 2.0

CLM-2095

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

1.1. Product identifier

Product form	:	Substance
Substance name	:	ISOVALERIC ACID (1-13C, 99%)
EC-No.	:	503-74-2 (Unlabeled)
CAS-No.	:	503-74-2 (Unlabeled)
Product code	:	CLM-2095
Formula	:	*CC4H10O2
Synonyms	:	3-Methylbutanoic acid, 3-Methylbutyric acid

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

1.2.1. Relevant identified uses

Main use category	:	Professional use
Industrial/Professional use spec	:	For professional use only

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000
cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)
International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Skin Corr. 1A H314

Eye Dam. 1 H318

Full text of hazard classes and H-statements : see section 16

Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

C; R35
Xi; R41
Xi; R39

Full text of R-phrases: see section 16

GHS-US classification

Flam. Liq. 4 H227
Skin Corr. 1A H314
Eye Dam. 1 H318

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :

GHS05

Signal word (CLP) : Danger

Hazard statements (CLP) : H314 - Causes severe skin burns and eye damage

Precautionary statements (CLP) : P260 - Do not breathe dust, fume, gas, mist, spray, vapors.
P264 - Wash Both hands thoroughly after handling.
P280 - Wear protective clothing, protective gloves.
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 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 - Immediately call a POISON CENTER or doctor.

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS05

Signal word (GHS-US) : Danger

Hazard statements (GHS-US) : H227 - Combustible liquid
H314 - Causes severe skin burns and eye damage
H318 - Causes serious eye damage

Precautionary statements (GHS-US) : P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking.
P260 - Do not breathe dust, fume, gas, mist, spray, vapors.
P264 - Wash Both hands thoroughly after handling.
P280 - Wear protective clothing, protective gloves.
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 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a poison center or doctor
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)
P363 - Wash contaminated clothing before reuse.
P370+P378 - In case of fire: Use Alcohol resistant foam, Carbon dioxide, Dry chemical, Water spray to extinguish.
P403+P235 - Store in a well-ventilated place. Keep cool.
P405 - Store locked up.
P501 - Dispose of contents/container to Comply with applicable regulations

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
ISOVALERIC ACID (1-13C, 99%)	(CAS-No.) 503-74-2 (Unlabeled) (EC-No.) 503-74-2 (Unlabeled)	100	C; R35 Xi; R41 Xi; R39

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
ISOVALERIC ACID (1-13C, 99%)	(CAS-No.) 503-74-2 (Unlabeled) (EC-No.) 503-74-2 (Unlabeled)	100	Skin Corr. 1A, H314 Eye Dam. 1, H318

Full text of R- and H- phrases: see section 16

Name	Product identifier	%	GHS-US classification
ISOVALERIC ACID (1-13C, 99%) (Main constituent)	(CAS-No.) 503-74-2 (Unlabeled)	100	Flam. Liq. 4, H227 Skin Corr. 1A, H314 Eye Dam. 1, H318

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

First-aid measures after inhalation : If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.

First-aid measures after skin contact : Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

First-aid measures after eye contact : Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

First-aid measures after ingestion : 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

Symptoms/effects after inhalation : May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

Symptoms/effects after skin contact : May be harmful if absorbed through the skin. Causes skin burns.

Symptoms/effects after eye contact : Causes eye burns.

Symptoms/effects after ingestion : May be harmful if swallowed.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

5.2. Special hazards arising from the substance or mixture

No additional information available

5.3. Advice for firefighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Use water spray to cool unopened containers.

6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment. Avoid breathing vapors, 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.

6.1.2. For emergency responders

No additional information available

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 material for containment and cleaning up

For containment : Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

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

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Liquid
Appearance	:	Liquid, clear
Molecular mass	:	103.12 g/mol (Lableed)
Color	:	Colorless to yellow
Odor	:	Penetrating odor
Odor threshold	:	No data available
pH	:	No data available
Relative evaporation rate (butyl acetate=1)	:	No data available
Melting point	:	-29 °C (-20 °F)
Freezing point	:	No data available
Boiling point	:	175 - 177 °C (347 - 351 °F)
Flash point	:	74 °C (165 °F)
Auto-ignition temperature	:	No data available
Decomposition temperature	:	No data available
Flammability (solid, gas)	:	No data available
Vapor pressure	:	0.507 hPa (0.380 mmHg) at 20 °C (68 °F)
Relative vapor density at 20 °C	:	No data available
Relative density	:	No data available
Specific gravity / density	:	0.925 g/cm³ at 20 °C (68 °F)
Solubility	:	No data available
Log Pow	:	No data available
Log Kow	:	No data available
Viscosity, kinematic	:	No data available

Viscosity, dynamic	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	No data available
Explosion limits	:	No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Avoid Heat, Flames and Sparks.

10.5. Incompatible materials

Bases, Oxidizing agents, Reducing agents.

10.6. Hazardous decomposition products

Formed under fire conditions: Carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

ISOVALERIC ACID (1-13C, 99%) (503-74-2 (Unlabeled))	
LD50 oral rat	> 2000 mg/kg
LD50 dermal rabbit	3560 mg/kg
ATE CLP (dermal)	3560.000 mg/kg body weight

Skin corrosion/irritation	:	Causes severe skin burns and eye damage. Rabbit - Result: Causes burns - 24 hours
Serious eye damage/irritation	:	Causes serious eye damage.
Respiratory or skin sensitization	:	Not classified
Germ cell mutagenicity	:	Not classified
Carcinogenicity	:	Not classified
Reproductive toxicity	:	Not classified
Specific target organ toxicity – single exposure	:	Not classified
Specific target organ toxicity – repeated exposure	:	Not classified
Aspiration hazard	:	Not classified
Potential Adverse human health effects and symptoms	:	Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract, eyes, and skin. Spasm, inflammation and edema of the larynx, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, cough, wheezing, laryngitis, shortness of breath, headache, nausea, vomiting. The chemical, physical, and toxicological properties have not been thoroughly investigated. This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	:	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Symptoms/effects after skin contact	:	May be harmful if absorbed through the skin. Causes skin burns.
Symptoms/effects after eye contact	:	Causes eye burns.
Symptoms/effects after ingestion	:	May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

UN-No.(DOT) : 3265

DOT NA no. UN3265

14.2. UN proper shipping name

Proper Shipping Name (DOT) : Corrosive liquid, acidic, organic, n.o.s.

Class (DOT) : 8 - Class 8 - Corrosive material 49 CFR 173.136

Hazard labels (DOT) : 8 - Corrosive

DOT Symbols : G - Identifies PSN requiring a technical name

Packing group (DOT) : II - Medium Danger

DOT Special Provisions (49 CFR 172.102) : B2 - MC 300, MC 301, MC 302, MC 303, MC 305, and MC 306 and DOT 406 cargo tanks are not authorized.
IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized.
T11 - 6 178.274(d)(2) Normal..... 178.275(d)(3)
TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
TP27 - A portable tank having a minimum test pressure of 4 bar (400 kPa) may be used provided the calculated test pressure is 4 bar or less based on the MAWP of the hazardous material, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.

DOT Packaging Exceptions (49 CFR 173.xxx) : 154

DOT Packaging Non Bulk (49 CFR 173.xxx) : 202

DOT Packaging Bulk (49 CFR 173.xxx) : 242

Marine pollutant : No

14.3. Additional information

Other information : No supplementary information available.

Overland transport

Packing group (ADR)	:	II
Class (ADR)	:	8 - Corrosive substances
Hazard identification number (Kemler No.)	:	80
Classification code (ADR)	:	C3
Hazard labels (ADR)	:	8 - Corrosive substances

Orange plates :

Tunnel restriction code (ADR)	:	E
Limited quantities (ADR)		1l
EAC	:	2X
APP	:	B
Excepted quantities (ADR)	:	E2

Transport by sea

DOT Vessel Stowage Location	:	B - (i) The material may be stowed ‘‘on deck’’ or ‘‘under deck’’ on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) ‘‘On deck only’’ on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.
DOT Vessel Stowage Other	:	40 - Stow ‘‘clear of living quarters’’
MFAG-No	:	153

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	:	1 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	:	30 L
Civil Aeronautics Law	:	Corrosive substances

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

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

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

ISOVALERIC ACID (1-13C, 99%) (503-74-2 (Unlabeled))	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302
SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313

15.2. International regulations

CANADA

No additional information available

15.2.1. National regulations

No additional information available

15.3. US State regulations

ISOVALERIC ACID (1-13C, 99%)(503-74-2 (Unlabeled))	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	RTK - U.S. - Massachusetts - Right To Know List RTK - U.S. - Pennsylvania - RTK (Right to Know) List RTK - U.S. - New Jersey - Right to Know Hazardous Substance List

SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

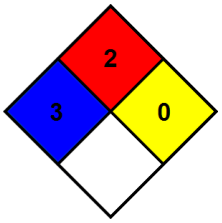
Full text of R-, H- and EUH-phrases:

Eye Dam. 1	Serious eye damage/eye irritation Category 1
Skin Corr. 1A	Skin corrosion/irritation Category 1A
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
R35	Causes severe burns
R39	Danger of very serious irreversible effects
R41	Risk of serious damage to eyes
C	Corrosive
Xi	Irritant

NFPA health hazard : 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard : 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given

Flammability : 2 Moderate Hazard

Physical : 0 Minimal Hazard

CIL Substance SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product