OCTANOIC ACID (1,2,3,4-13C4, 99%)

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 16/02/2011 Revision date: 27/07/2016 Supersedes: 16/02/2011 Version: 3.0

CLM-2721

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

1.1. Product identifier

Product form	:	Substance
Substance name	:	OCTANOIC ACID (1,2,3,4-13C4, 99%)
EC no	:	204-677-5 (Unlabeled)
CAS No	:	124-07-2 (Unlabeled)
Product code	:	CLM-2721
Formula	:	CH3(CH2)3(*CH2)3*COOH
Synonyms	:	Caprylic acid / Acid C8

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 H-phrases: see section 16

Classification according to Directive 67/548/EEC or 1999/45/EC

C; R35
Xi; R41
Xi; R39
R52

Full text of R-phrases: see section 16

Classification (GHS-US)

Skin Corr. 1A H314
Eye Dam. 1 H318
Aquatic Acute 3 H402

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 spray, mist
P264 - Wash both hands thoroughly after handling
P280 - Wear eye protection, face protection, protective gloves, protective clothing
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/doctor/…

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS05

Signal word (GHS-US) : Danger

Hazard statements (GHS-US) : H314 - Causes severe skin burns and eye damage
H318 - Causes serious eye damage
H402 - Harmful to aquatic life

Precautionary statements (GHS-US) : P260 - Do not breathe mist, spray
P264 - Wash Both hands thoroughly after handling
P273 - Avoid release to the environment
P280 - Wear eye protection, face protection, protective clothing, protective gloves
P301+P330+P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
P303+P361+P353 - IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower
P304+P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position 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/physician
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)
P363 - Wash contaminated clothing before reuse
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
OCTANOIC ACID (1,2,3,4-13C4, 99%) (Main constituent)	(CAS No) 124-07-2 (Unlabeled) (EC no) 204-677-5 (Unlabeled)	100	C; R35 Xi; R41 Xi; R39 R52

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
OCTANOIC ACID (1,2,3,4-13C4, 99%) (Main constituent)	(CAS No) 124-07-2 (Unlabeled) (EC no) 204-677-5 (Unlabeled)	100	Skin Corr. 1A, H314 Eye Dam. 1, H318

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

Name	Product identifier	%	Classification (GHS-US)
OCTANOIC ACID (1,2,3,4-13C4, 99%) (Main constituent)	(CAS No) 124-07-2 (Unlabeled)	100	Skin Corr. 1A, H314 Eye Dam. 1, H318 Aquatic Acute 3, H402

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

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

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

Symptoms/injuries after eye contact : Causes eye burns.

Symptoms/injuries 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 : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Special hazards arising from the substance or mixture

No additional information available

5.3. Advice for firefighters

Firefighting instructions : Wear self contained breathing apparatus for fire fighting if necessary.

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

6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation. Evacuate personnel to safe area.

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 : Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

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 inhalation of vapour or mist. Normal measures for preventive fire protection.

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	:	Keep container tightly closed in a cool, dry and well-ventilated place.
Storage conditions	:	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

Appropriate engineering controls	:	Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
Personal protective equipment	:	Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Materials for protective clothing	:	Wear suitable protective clothing and gloves.
Hand protection	:	Wear suitable protective clothing and gloves.
Eye protection	:	Wear safety glasses with side shields (or goggles) and a face shield.
Skin and body protection	:	Wear complete suit protecting against chemicals according to concentration and amount of substance.
Respiratory protection	:	When appropriate, use NIOSH/CEN approved respirator.
Environmental exposure controls	:	Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Liquid
Appearance	:	Clear, viscous liquid.
Molecular mass	:	148.18 g/mol (Labeled)
Color	:	Light yellow.
Odor	:	No data available
Odor threshold	:	No data available
pH	:	3.5 at 0.5 g/l
Relative evaporation rate (butyl acetate=1)	:	No data available
Melting point	:	15 - 17 °C (59 - 63°F) - lit.
Freezing point	:	No data available
Boiling point	:	237 °C (459 °F) - lit.
Flash point	:	> 110 °C (> 230 °F) - closed cup
Self ignition temperature	:	> 300 °C (> 572 °F)
Decomposition temperature	:	No data available
Flammability (solid, gas)	:	No data available
Vapor pressure	:	13 hPa (10 mmHg) at 124 °C (255 °F); 1 hPa (1 mmHg) at 78 °C (172 °F)
Relative vapor density at 20 °C	:	4.98 - (Air = 1.0)
Relative density	:	No data available
Density	:	0.91 g/ml at 25 °C (77 °F)
Solubility	:	Water: 0.68 g/l at 20 °C (68 °F)
Log Pow	:	3.05
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
Explosive 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

Not available.

10.5. Incompatible materials

Bases, Oxidizing agents, Reducing agents.

10.6. Hazardous decomposition products

carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
LD50 oral rat	> 2000 mg/kg male and female (OECD Test Guideline 401)
LD50 dermal rabbit	> 5000 mg/kg
ATE (oral)	10080.000 mg/kg body weight

Skin corrosion/irritation : Skin - Rabbit Result: Causes burns. (OECD Test Guideline 404)
No data available
pH: 3.5 at 0.5 g/l

Serious eye damage/irritation : Eyes - rabbit Result: Irritating to eyes.
No data available
pH: 3.5 at 0.5 g/l

Respiratory or skin sensitization : Not available
No data available

Germ cell mutagenicity : Not available

Carcinogenicity : Not classified

Reproductive toxicity : Not available

Specific target organ toxicity (single exposure) : Not classified
No data available

Specific target organ toxicity (repeated exposure) : Not classified
No data available

Aspiration hazard : Not classified

Potential Adverse human health effects and symptoms : Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin Cough, Shortness of breath, Nausea. Headache.

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

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

Symptoms/injuries after eye contact : Causes eye burns.

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

SECTION 12: Ecological information

12.1. Toxicity

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
LC50 fish 1	22 mg/l static test - Lepomis machrochirus (Bluegill sunfish) - 96 h
EC50 Daphnia 1	550 mg/l Immobilization - Daphnia magna (Water flea) - 48 h (OECD Test Guideline 201)
EC50 other aquatic organisms 1	31 mg/l Growth Inhibition - Pseudokirchneriella subcapitata (green algae) - 72 h (OECD Test Guideline 201)

12.2. Persistence and degradability

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
Persistence and degradability	Aerobic - exposure time: 28 d.
Biodegradation	51.6 % Not readily biodegradable (OECD Test Guideline 301B)

12.3. Bioaccumulative potential

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
Log Pow	3.05
Bioaccumulative potential	Not available.

12.4. Mobility in soil

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
Ecology - soil	Not available.

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : An environmental hazard cannot be excluded in the event of an unprofessional handling or disposal. Harmful to aquatic life.

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.

Waste disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Ecology - waste materials : Dispose of as unused product.

SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

14.1. UN number

UN-No.(DOT) : 3265

DOT NA no. UN3265

14.2. UN proper shipping name

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

Department of Transportation (DOT) Hazard Classes : 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) : III - Minor Danger

DOT Special Provisions (49 CFR 172.102) : IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). 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, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).
T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3)
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = 97 / 1 + a (tr - tf) Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
TP28 - A portable tank having a minimum test pressure of 2.65 bar (265 kPa) may be used provided the calculated test pressure is 2.65 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) : 203

DOT Packaging Bulk (49 CFR 173.xxx) : 241

Marine pollutant : No

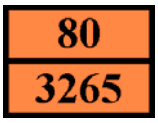
14.3. Additional information

Other information : No supplementary information available.

Overland transport

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

Orange plates :



Tunnel restriction code : E
Limited quantities (ADR) 5L
EAC : 2X
APP : B
Excepted quantities (ADR) : E1

Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed ''on deck'' or ''under deck'' on a cargo vessel and on a passenger vessel.
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) : 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 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

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

15.2. International regulations

CANADA

OCTANOIC ACID (1,2,3,4-13C4, 99%) (124-07-2 (Unlabeled))
Listed on the Canadian DSL (Domestic Substances List) inventory.

15.2.1. National regulations

No additional information available

15.3. US State regulations

OCTANOIC ACID (1,2,3,4-13C4, 99%)(124-07-2 (Unlabeled))	
State or local regulations	U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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.

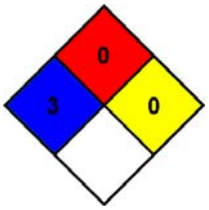
Full text of R-, H- and EUH-phrases::

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
R52	Harmful to aquatic organisms
C	Corrosive
Xi	Irritant

NFPA health hazard : 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard : 0 - Materials that will not burn.

NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

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

Flammability : 0 Minimal Hazard

Physical : 0 Minimal Hazard

CIL Multi-Solvent Mixture 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