DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 4/13/2016 Revision date: 5/1/2023 Supersedes: 3/8/2023 Version: 2.1

SECTION 1: Identification

1.1. Identification

Product form	:	Substance
Substance name	:	DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY
CAS-No.	:	112-85-6
Product code	:	CLM-9909
Formula	:	CH3(CH2)15(*CH2)5*COOH
Synonyms	:	Behenic acid

1.2. Recommended use and restrictions on use

No additional information available

1.3. Supplier

Cambridge Isotope Laboratories, Inc.
50 Frontage Rd
01810
ANDOVER, MA, 01810
USA
T 1-800-322-1174
cilsales@isotope.com - www.isotope.com

1.4. Emergency telephone number

Emergency number	:	1-703-741-5970 Chemtrec 1-800-424-9300 24 hours

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Not classified

2.2. GHS Label elements, including precautionary statements

GHS US labeling

No labeling applicable

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS US classification
DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (Main constituent)	CAS-No.: 112-85-6	100	Not classified

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

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : If breathed in, move person into fresh air. If not breathing, give artificial respiration.
First-aid measures after skin contact : Wash off with soap and plenty of water.
First-aid measures after eye contact : Flush eyes with water as a precaution.
First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Rinse mouth with water.

4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms : 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. May cause respiratory tract irritation.
Symptoms/effects after skin contact : May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact : May cause eye irritation.
Symptoms/effects after ingestion : May be harmful if swallowed.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Specific hazards arising from the chemical

No additional information available

5.3. Special protective equipment and precautions for fire-fighters

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 : Avoid dust formation. Avoid breathing vapors, mist or gas.

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 : Take up mechanically (sweeping, shoveling) and collect in suitable container for disposal.
Methods for cleaning up : Sweep up and shovel. 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

Precautions for safe handling : Provide appropriate exhaust ventilation at places where dust is formed.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store at room temperature away from light and moisture.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)

No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.
Environmental exposure controls : Avoid release to the environment.

8.3. Individual protection measures/Personal protective equipment

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:

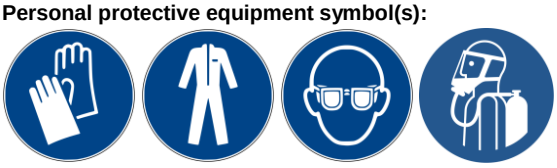
Wear eye protection. Chemical goggles or face shield with safety glasses

Skin and body protection:

Wear suitable protective clothing, gloves and eye/face protection

Respiratory protection:
In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator

Personal protective equipment symbol(s):



SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Solid
Appearance	:	Solid.
Color	:	White
Odor	:	No data available
Odor threshold	:	No data available
pH	:	5.64 at 1 g/l at 28 °C (82 °F)
Melting point	:	72 – 80 °C (162 - 176 °F) - lit.
Freezing point	:	No data available
Boiling point	:	300 °C (572 °F) at 1,013 hPa (760 mmHg)
Flash point	:	No data available
Relative evaporation rate (butyl acetate=1)	:	No data available
Flammability (solid, gas)	:	No data available
Vapor pressure	:	No data available
Relative vapor density at 20°C	:	No data available
Relative density	:	0.54 g/cm3 at 25 °C (77 °F)
Molecular mass	:	346.54 g/mol (Labeled)
Solubility	:	Water: 0.15 g/l
Partition coefficient n-octanol/water (Log Pow)	:	0.48 at 25 °C (77 °F)
Auto-ignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, kinematic	:	No data available
Viscosity, dynamic	:	No data available
Explosion limits	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	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

No additional information 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 (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)	
LD50 oral rat	> 2000 mg/kg (OECD Test Guideline 401)

Skin corrosion/irritation : Not classified
pH: 5.64 at 1 g/l at 28 °C (82 °F)
Serious eye damage/irritation : Not classified
pH: 5.64 at 1 g/l at 28 °C (82 °F)
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
STOT-single exposure : Not classified
STOT-repeated exposure : Not classified
Aspiration hazard : Not classified
Viscosity, kinematic : No data available
Potential Adverse human health effects and symptoms : 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. May cause respiratory tract irritation.
Symptoms/effects after skin contact : May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact : May cause eye irritation.
Symptoms/effects after ingestion : May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)	
LC50 - Fish [1]	> 5 mg/l semi-static test LC50 - Oryzias latipes (Orange-red killifish) - 96 h

12.2. Persistence and degradability

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)	
Biodegradation	79 – 86 % aerobic Biochemical oxygen demand - Exposure time 28 d - Readily biodegradable.

12.3. Bioaccumulative potential

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)	
Partition coefficient n-octanol/water (Log Pow)	0.48 at 25 °C (77 °F)

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Other adverse effects : Disposal must be done according to official regulations.

SECTION 13: Disposal considerations

13.1. Disposal methods

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

Product/Packaging disposal recommendations : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Ecology - waste materials : Dispose of as unused product.

SECTION 14: Transport information

In accordance with DOT / TDG / IMDG / IATA

14.1. UN number

Not regulated for transport

14.2. UN proper shipping name

Proper Shipping Name (DOT) : Not applicable
Proper Shipping Name (TDG) : Not applicable
Proper Shipping Name (IMDG) : Not applicable
Proper Shipping Name (IATA) : Not applicable

14.3. Transport hazard class(es)

DOT
Transport hazard class(es) (DOT) : Not applicable

TDG
Transport hazard class(es) (TDG) : Not applicable

IMDG
Transport hazard class(es) (IMDG) : Not applicable

IATA
Transport hazard class(es) (IATA) : Not applicable

14.4. Packing group

Packing group (DOT) : Not applicable
Packing group (TDG) : Not applicable
Packing group (IMDG) : Not applicable
Packing group (IATA) : Not applicable

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

Special transport precautions : DOT/IMDG/IATA: Not dangerous goods

DOT
No data available

TDG
No data available

IMDG
No data available

IATA
No data available

14.7. 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

Commercial status of components according to the United States Environmental Protection Agency's Toxic Substances Control Act (TSCA):

Name	CAS-No.	Listing	Commercial status	Flags
DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY	112-85-6	Not present	-	

15.2. International regulations

CANADA

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)
Not listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)
CAUTION: This material is supplied for research and development purposes subject to the R&D exemption under TSCA, 40 CFR 720.36, and must meet the requirements of the exemption, including supervision by a "technically qualified individual" as defined by 40 CFR 720.3(ee). The use of this material for "commercial purposes" as defined by 40 CFR 720.3(r) is not permitted in the United States.

15.3. US State regulations

DOCOSANOIC ACID (1,2,3,4,5,6-13C6, 99%) 95% CHEMICAL PURITY (112-85-6)	
State or local regulations	U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

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Revision date : 05/01/2023

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.

Safety Data Sheet (SDS), USA

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.