



CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 5/21/2015 Revision date: 11/17/2023 Supersedes: 8/14/2018 Version: 2.0

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL
Product code : CLM-514-S

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

Flammable liquids Category 2	H225	Highly flammable liquid and vapor
Acute toxicity (oral) Category 3	H301	Toxic if swallowed
Acute toxicity (dermal) Category 3	H311	Toxic in contact with skin
Acute toxicity (inhalation) Category 3	H331	Toxic if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Specific target organ toxicity (single exposure) Category 1	H370	Causes damage to organs (brain, heart, kidneys, liver, eyes) (Dermal, Inhalation, oral)

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) :

Danger

Hazard statements (GHS US) :

H225 - Highly flammable liquid and vapor
H301+H311+H331 - Toxic if swallowed, in contact with skin or if inhaled
H315 - Causes skin irritation

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Precautionary statements (GHS US)

H319 - Causes serious eye irritation
H370 - Causes damage to organs (brain, heart, kidneys, liver, eyes) (Dermal, Inhalation, oral)
: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. hot surfaces, heat, open flames, sparks
P233 - Keep container tightly closed.
P240 - Ground/Bond container and receiving equipment.
P241 - Use explosion-proof electrical, ventilating, lighting equipment.
P242 - Use only non-sparking tools.
P243 - Take precautionary measures against static discharge.
P260 - Do not breathe dust, fume, gas, mist, spray, vapors.
P261 - Avoid breathing dust, fume, gas, spray, mist, vapors.
P264 - Wash Both hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear eye protection, face protection, protective clothing, protective gloves.
P301+P310 - If swallowed: Immediately call a poison center or doctor.
P302+P352 - If on skin: Wash with plenty of water.
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.
P311 - Call a poison center or doctor.
P312 - Call a poison center or doctor if you feel unwell.
P321 - Specific treatment (see Hazard pictograms (CLP) on this label).
P330 - Rinse mouth.
P332+P313 - If skin irritation occurs: Get medical advice/attention.
P337+P313 - If eye irritation persists: Get medical advice/attention.
P361 - Take off immediately all contaminated clothing.
P362 - Take off contaminated clothing and wash before reuse.
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+P233 - Store in a well-ventilated place. Keep container tightly closed.
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 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

Not applicable

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3.2. Mixtures

Name	Product identifier	%	GHS US classification
100% METHANOL UNLABELED	CAS-No.: 67-56-1	99.987	Flam. Liq. 2, H225 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Inhalation:vapour), H331 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 1, H370
CAFFEINE (TRIMETHYL-13C3, 99%)	CAS-No.: 78072-66-9	0.013	Acute Tox. 4 (Oral), H302

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

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general	: If medical advice is needed, have product container or label at hand. Call a physician immediately. Evacuate danger area.
First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Call a doctor.
First-aid measures after skin contact	: Rinse skin with water/shower. Take immediately victim to hospital. Remove/Take off immediately all contaminated clothing. If skin irritation occurs: Get medical advice/attention.
First-aid measures after eye contact	: Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth. Call a physician immediately.

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. Effects due to Ingestion may include: Headache. Dizziness. Drowsiness. metabolic acidosis. Coma. May be fatal if swallowed and enters airways. If swallowed there is a risk of blindness. Effects on humans. stomach.
Symptoms/effects	: Causes damage to organs (Eyes, heart, liver, kidneys, central nervous system, Skin) (in contact with skin, if inhaled, if swallowed).
Symptoms/effects after inhalation	: Toxic if inhaled.
Symptoms/effects after skin contact	: Toxic in contact with skin. Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: Toxic if swallowed.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: Dry powder. Dry sand.
Unsuitable extinguishing media	: Do not use a heavy water stream.

5.2. Specific hazards arising from the chemical

Fire hazard	: Highly flammable liquid and vapor.
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Hazardous decomposition products in case of fire : Toxic fumes may be released.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions : Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing. Wear recommended personal protective equipment.
Other information : Use water spray to cool exposed surfaces.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Wear respiratory protection. Do not breathe dust, mist, gas, spray, vapors, fume. Avoid contact with skin, eyes and clothing. Ventilate spillage area. Remove all sources of ignition. No open flames, no sparks, and no smoking. Ensure adequate air ventilation. Special attention should be given to low areas/pits where flammable vapors can accumulate.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

For containment : Dike and contain spill. For large spills, confine the spill in a dike and charge it with wet sand or earth for subsequent safe disposal. Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal.
Methods for cleaning up : Take up liquid spill into absorbent material. Notify authorities if product enters sewers or public waters. This material and its container must be disposed of in a safe way, and as per local legislation.
Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Flammable vapors may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Do not breathe dust, fume, gas, spray, vapors, mist. Do not get in eyes, on skin, or on clothing. Use only outdoors or in a well-ventilated area.
Hygiene measures : Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Ground/bond container and receiving equipment. Use explosion-proof electrical equipment.

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Storage conditions : Store at room temperature away from light and moisture.
Incompatible materials : Heat sources.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
USA - ACGIH - Occupational Exposure Limits	
ACGIH OEL TWA [ppm]	200 ppm Basis: USA. ACGIH Threshold Limit Values (TLV)
ACGIH OEL STEL [ppm]	250 ppm Basis: USA. ACGIH Threshold Limit Values (TLV)
Remark (ACGIH)	Headache. Nausea. Dizziness. Eye damage. Substances for which there is a Biological Exposure Index or Indices (see BEI section). Danger of cutaneous absorption.
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
USA - ACGIH - Biological Exposure Indices	
BEI	15 mg/l Urine Basis: ACGIH - Biological Exposure Indices (BEI)
Remark	End of shift (As soon as possible after exposure ceases)
USA - OSHA - Occupational Exposure Limits	
OSHA PEL TWA [1]	260 mg/m ³ Basis: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL TWA [2]	200 ppm Basis: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL STEL [1]	325 mg/m ³ Basis: USA. OSHA - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL STEL [2]	250 ppm Basis: USA. OSHA - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL C [ppm]	1000 ppm California permissible exposure limits for chemical contaminants (Title 8, Article 107)
Remark (OSHA)	The value in mg/m ³ is approximate. Skin notation.
USA - NIOSH - Occupational Exposure Limits	
NIOSH REL TWA	260 mg/m ³ Basis: NIOSH Recommended Exposure Limits
NIOSH REL TWA [ppm]	200 ppm Basis: NIOSH Recommended Exposure Limits
NIOSH REL STEL	325 mg/m ³ Basis: NIOSH Recommended Exposure Limits
NIOSH REL STEL [ppm]	250 ppm Basis: NIOSH Recommended Exposure Limits
Remark (NIOSH)	Potential for dermal absorption.
CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
No additional information available	
100% METHANOL UNLABELED (67-56-1)	
USA - ACGIH - Occupational Exposure Limits	
ACGIH OEL TWA [ppm]	200 ppm Basis: USA. ACGIH Threshold Limit Values (TLV)

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100% METHANOL UNLABELED (67-56-1)	
ACGIH OEL STEL [ppm]	250 ppm Basis: USA. ACGIH Threshold Limit Values (TLV)
Remark (ACGIH)	Headache. Nausea. Dizziness. Eye damage. Substances for which there is a Biological Exposure Index or Indices (see BEI section). Danger of cutaneous absorption.
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
USA - ACGIH - Biological Exposure Indices	
BEI	15 mg/l Urine Basis: ACGIH - Biological Exposure Indices (BEI)
Remark	End of shift (As soon as possible after exposure ceases)
USA - OSHA - Occupational Exposure Limits	
OSHA PEL TWA [1]	260 mg/m ³ Basis: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL TWA [2]	200 ppm Basis: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL STEL [1]	325 mg/m ³ Basis: USA. OSHA - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL STEL [2]	250 ppm Basis: USA. OSHA - Table Z-1 Limits for Air Contaminants - 1910.1000. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
OSHA PEL C [ppm]	1000 ppm California permissible exposure limits for chemical contaminants (Title 8, Article 107)
Remark (OSHA)	The value in mg/m ³ is approximate. Skin notation.
USA - NIOSH - Occupational Exposure Limits	
NIOSH REL TWA	260 mg/m ³ Basis: NIOSH Recommended Exposure Limits
NIOSH REL TWA [ppm]	200 ppm Basis: NIOSH Recommended Exposure Limits
NIOSH REL STEL	325 mg/m ³ Basis: NIOSH Recommended Exposure Limits
NIOSH REL STEL [ppm]	250 ppm Basis: NIOSH Recommended Exposure Limits
Remark (NIOSH)	Potential for dermal absorption.

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

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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	: Liquid
Appearance	: Liquid.
Color	: Colorless
Odor	: Pungent
Odor threshold	: No data available
pH	: No data available
Melting point	: -98 °C (-144 °F)
Freezing point	: No data available
Boiling point	: 64.7 °C (148.5 °F)
Flash point	: 9.7 °C (49.5 °F) - closed cup
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: 130.3 hPa (97.7 mmHg) at 20 °C (68 °F); 169.27 hPa (126.96 mmHg) at 25 °C (77 °F)
Vapor pressure at 50°C	: 546.6 hPa (410 mmHg) at 50 °C (122 °F)
Relative vapor density at 20°C	: 1.11
Relative density	: No data available
Density	: 0.791 g/ml at 25 °C (77 °F)
Molecular mass	: 32.04 g/mol
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: -0.77
Auto-ignition temperature	: 455 °C (851 °F) at 1,013 hPa (760 mmHg)
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: 6 – 36 % (V)
Explosive properties	: Product is not explosive.
Oxidizing properties	: Non oxidizing material according to EC criteria.

9.2. Other information

No additional information available

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SECTION 10: Stability and reactivity

10.1. Reactivity

Vapors may form flammable mixture with air. Highly flammable liquid and vapor.

10.2. Chemical stability

See storage and expiration date on CoA.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

10.5. Incompatible materials

Acid anhydrides. Acid chlorides. Oxidizing agent. Alkali Metal Amides. Reducing agents. Acids.

10.6. Hazardous decomposition products

Carbon oxides (CO, CO2).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Toxic if swallowed.
Acute toxicity (dermal) : Toxic in contact with skin.
Acute toxicity (inhalation) : Toxic if inhaled.

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
LD50 oral rat	1187 – 2769 mg/kg
LD50 dermal rabbit	17100 mg/kg
LC50 Inhalation - Rat	128.2 mg/l/4h ; 87.6 mg/l - 6 h
ATE US (oral)	100 mg/kg body weight
ATE US (dermal)	300 mg/kg body weight
ATE US (gases)	700 ppmV/4h
ATE US (vapors)	3 mg/l/4h
ATE US (dust, mist)	0.5 mg/l/4h
Additional data	LDLO, oral, human: 143 mg/kg Remarks: Lungs, Thorax, or Respiration: Dyspnea. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea.

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
LD50 oral rat	367.7 mg/kg - male and female (OECD Test Guideline 401)
LD50 dermal	> 2000 mg/kg - male and female
LC50 Inhalation - Rat	4.94 mg/l - male and female (Calculation method)
ATE US (oral)	500 mg/kg body weight

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100% METHANOL UNLABELED (67-56-1)	
LD50 oral rat	1187 – 2769 mg/kg
LD50 dermal rabbit	17100 mg/kg
LC50 Inhalation - Rat	128.2 mg/l/4h ; 87.6 mg/l - 6 h
ATE US (oral)	100 mg/kg body weight
ATE US (dermal)	300 mg/kg body weight
ATE US (vapors)	3 mg/l/4h
ATE US (dust, mist)	128.2 mg/l/4h
LDLO, oral, human	143 mg/kg Remarks: Lungs, Thorax, or Respiration: Dyspnea. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea.

Skin corrosion/irritation : Causes skin irritation.

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
pH	5.5 – 6.5 at 10 g/l at 20 °C (68 °F)

Serious eye damage/irritation : Causes serious eye irritation.

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
pH	5.5 – 6.5 at 10 g/l at 20 °C (68 °F)

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
IARC group	3 - Not classifiable

100% METHANOL UNLABELED (67-56-1)	
National Toxicology Program (NTP) Status	No component of this product present at levels greater than or equal to 0.1% is identifiable as probable, possible, or confirmed human carcinogen by IARC.

Reproductive toxicity : Not classified

STOT-single exposure : Causes damage to organs (brain, heart, kidneys, liver, eyes) (Dermal, Inhalation, oral).

100% METHANOL UNLABELED (67-56-1)	
STOT-single exposure	Causes damage to organs (eyes, kidneys, liver, heart, central nervous system) (Dermal, Inhalation, oral).

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. Effects due to Ingestion may include: Headache. Dizziness. Drowsiness. metabolic acidosis. Coma. May be fatal if swallowed and enters airways. If swallowed there is a risk of blindness. Effects on humans. stomach.

Symptoms/effects : Causes damage to organs (Eyes, heart, liver, kidneys, central nervous system, Skin) (in contact with skin, if inhaled, if swallowed).

Symptoms/effects after inhalation : Toxic if inhaled.

Symptoms/effects after skin contact : Toxic in contact with skin. Causes skin irritation.

Symptoms/effects after eye contact : Causes serious eye irritation.

Symptoms/effects after ingestion : Toxic if swallowed.

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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.

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
LC50 - Fish [1]	15400 mg/l mortality LC50 - Lepomis macrochirus (Bluegill) - 96 h
EC50 - Crustacea [1]	> 10000 mg/l Daphnia magna (Water flea) - 48 h
EC50 - Crustacea [2]	22000 mg/l Growth inhibition EC50 - Scenedesmus capricornutum (fresh water algae) - 96 h
NOEC (acute)	7900 mg/l Oryzias latipes - 200 h

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
LC50 - Fish [1]	87 mg/l - Leuciscus idus (Golden orfe) - 96 h
EC50 - Crustacea [1]	182 mg/l static test - Daphnia magna (Water flea) - 48 h (DIN 38412)
ErC50 algae	Toxicity to algae static test - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

100% METHANOL UNLABELED (67-56-1)	
LC50 - Fish [1]	15400 mg/l mortality LC50 - Lepomis macrochirus (Bluegill) - 96 h
EC50 - Crustacea [1]	> 10000 mg/l Daphnia magna (Water flea) - 48 h
EC50 - Crustacea [2]	22000 mg/l Growth inhibition EC50 - Scenedesmus capricornutum (fresh water algae) - 96 h
NOEC (acute)	7900 mg/l Oryzias latipes - 200 h

12.2. Persistence and degradability

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
Biochemical oxygen demand (BOD)	600 – 1200 mg/g
Chemical oxygen demand (COD)	1420 mg/g
ThOD	1500 mg/g
Biodegradation	72 % - rapidly biodegradable aerobic - Exposure time 5 d

100% METHANOL UNLABELED (67-56-1)	
Biochemical oxygen demand (BOD)	600 – 1200 mg/g
Chemical oxygen demand (COD)	1420 mg/g
ThOD	1500 mg/g
Biodegradation	72 % - rapidly biodegradable aerobic - Exposure time 5 d

12.3. Bioaccumulative potential

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
BCF - Fish [1]	5 mg/l Cyprinus carpio (Carp) - 72 d at 20 °C
Bioconcentration factor (BCF REACH)	1
Partition coefficient n-octanol/water (Log Pow)	-0.77

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CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
Partition coefficient n-octanol/water (Log Pow)	-0.091 at 23 °C (73 °F)
100% METHANOL UNLABELED (67-56-1)	
BCF - Fish [1]	5 mg/l Cyprinus carpio (Carp) - 72 d at 20 °C
Bioconcentration factor (BCF REACH)	1
Partition coefficient n-octanol/water (Log Pow)	-0.77

12.4. Mobility in soil

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
Ecology - soil	Not degradable in the soil.
100% METHANOL UNLABELED (67-56-1)	
Ecology - soil	Not degradable in the soil.

12.5. Other adverse effects

Other adverse effects	: Avoid release to the environment. Disposal must be done according to official regulations.
Other information	: Stability in water: at 19 °C - (83 - 91%) - 72 h. Remarks: Hydrolyses on contact with water. Hydrolyses readily.

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

DOT NA No	: UN1230
UN-No. (TDG)	: UN1230
UN-No. (IMDG)	: 1230
UN-No. (IATA)	: 1230

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Methanol
Proper Shipping Name (TDG)	: METHANOL
Proper Shipping Name (IMDG)	: METHANOL
Proper Shipping Name (IATA)	: Methanol

14.3. Transport hazard class(es)

DOT	
Transport hazard class(es) (DOT)	: 3 (6.1)
Hazard labels (DOT)	: 3, 6.1

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TDG

Transport hazard class(es) (TDG) : 3 (6.1)
Hazard labels (TDG) : 3, 6.1



IMDG

Transport hazard class(es) (IMDG) : 3 (6.1)
Hazard labels (IMDG) : 3, 6.1



IATA

Transport hazard class(es) (IATA) : 3 (6.1)
Hazard labels (IATA) : 3, 6.1



14.4. Packing group

Packing group (DOT) : II
Packing group (TDG) : II
Packing group (IMDG) : II
Packing group (IATA) : II

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT
UN-No.(DOT) : UN1230
DOT Special Provisions (49 CFR 172.102) : 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.
T7 - 4 178.274(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.
DOT Packaging Exceptions (49 CFR 173.xxx) : 150

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DOT Packaging Non Bulk (49 CFR 173.xxx)	: 202
DOT Packaging Bulk (49 CFR 173.xxx)	: 242
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 1 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 60 L
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"

TDG

UN-No. (TDG)	: UN1230
TDG Special Provisions	: 43 - Despite section 2.1 of Part 2 (Classification), these dangerous goods are assigned to this classification based on human experience.
Explosive Limit and Limited Quantity Index	: 1 L
Excepted quantities (TDG)	: E2
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	: 1 L
Emergency Response Guide (ERG) Number	: 131

IMDG

Special provision (IMDG)	: 279
Limited quantities (IMDG)	: 1 L
Excepted quantities (IMDG)	: E2
Packing instructions (IMDG)	: P001
IBC packing instructions (IMDG)	: IBC02
Tank instructions (IMDG)	: T7
Tank special provisions (IMDG)	: TP2
EmS-No. (Fire)	: F-E - FIRE SCHEDULE Echo - NON-WATER-REACTIVE FLAMMABLE LIQUIDS
EmS-No. (Spillage)	: S-D - SPILLAGE SCHEDULE Delta - FLAMMABLE LIQUIDS
Stowage category (IMDG)	: B
Stowage and handling (IMDG)	: SW2
Flash point (IMDG)	: 12°C c.c.
Properties and observations (IMDG)	: Colourless, volatile liquid. Flashpoint: 12°C c.c. Explosive limits: 6% to 36.5% Miscible with water. Toxic if swallowed; may cause blindness. Avoid skin contact.
MFAG-No	: 131

IATA

PCA Excepted quantities (IATA)	: E2
PCA Limited quantities (IATA)	: Y341
PCA limited quantity max net quantity (IATA)	: 1L
PCA packing instructions (IATA)	: 352
PCA max net quantity (IATA)	: 1L
CAO packing instructions (IATA)	: 364
CAO max net quantity (IATA)	: 60L
Special provision (IATA)	: A113
ERG code (IATA)	: 3L

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

Not applicable

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SECTION 15: Regulatory information

15.1. US Federal regulations

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
CERCLA RQ	5000 lb
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 Delayed (chronic) health hazard

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
CAFFEINE (TRIMETHYL-13C3, 99%)	78072-66-9	Not present	-	
100% METHANOL UNLABELED	67-56-1	Present	Active	

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
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	Immediate (acute) health hazard Delayed (chronic) health hazard

100% METHANOL UNLABELED (67-56-1)	
CERCLA RQ	5000 lb
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 Delayed (chronic) health hazard

15.2. International regulations

CANADA

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL
Listed on the Canadian DSL (Domestic Substances List)

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)
Listed on the Canadian DSL (Domestic Substances List)

100% METHANOL UNLABELED (67-56-1)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

No additional information available

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15.3. US State regulations

CAFFEINE (TRIMETHYL-13C3, 99%) 100 UG/ML IN METHANOL	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	Yes
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List

100% METHANOL UNLABELED (67-56-1)					
U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significant risk level (NSRL)	Maximum allowable dose level (MADL)
No	Yes	No	No		

Component	State or local regulations
CAFFEINE (TRIMETHYL-13C3, 99%)(78072-66-9)	U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List
100% METHANOL UNLABELED(67-56-1)	U.S. - Massachusetts - Right To Know List; U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List

SECTION 16: Other information

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Revision date

: 11/17/2023

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.

Full text of H-phrases	
H225	Highly flammable liquid and vapor
H301	Toxic if swallowed
H302	Harmful if swallowed
H311	Toxic in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H331	Toxic if inhaled

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Full text of H-phrases	
H370	Causes damage to organs

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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.