SAFETY DATA SHEET

Version 6.8
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Iodomethane-$^{12}C,d_3$

Product Number : 296759
Brand : Aldrich
CAS-No. : 865-50-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319
Carcinogenicity (Category 2), H351
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word: Danger

Hazard Statements

H301 + H331	Toxic if swallowed or if inhaled.
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
H410	Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P261	Avoid breathing mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water.Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Vesicant., Rapidly absorbed through skin.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : iodo(2H3)methane
Methyl-12C,d3 iodide

Formula : $^{12}CD_3I$
Molecular weight : 144.95 g/mol
CAS-No. : 865-50-9
EC-No. : 231-159-6

Component	Classification	Concentration
iodomethane-d3		
	Acute Tox. 3; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 2; H301, H331, H312, H315, H319, H351, H335, H400, H411 M-Factor - Aquatic Acute: 1	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting

(only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Hydrogen iodide
Combustible.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage stability Recommended storage temperature
2 - 8 °C
Storage class
Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
iodomethane-d_3	865-50-9	TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		TWA	2 ppm 10 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen Potential for dermal absorption		
		TWA	5 ppm 28 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		PEL	2 ppm 10 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
required

Body Protection
protective clothing

Respiratory protection
Recommended Filter type: Filter type AX
The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.
required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/ range: -66.5 °C (-87.7 °F) - lit.
f)	Initial boiling point and boiling range	42 °C 108 °F - lit.
g)	Flash point	()No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or	Upper explosion limit: 66 %(V) Lower explosion limit: 8.5 %(V)

	explosive limits	
k)	Vapor pressure	544 hPa at 20 °C (68 °F) 1,660 hPa at 55 °C(131 °F)
l)	Vapor density	4.90 - (Air = 1.0)
m)	Density	2.33 g/mL at 25 °C (77 °F)2.33 g/cm3 at 25 °C (77 °F)
	Relative density	No data available
n)	Water solubility	14 g/l at 20 °C (68 °F)
o)	Partition coefficient: n-octanol/water	log Pow: 1.5 at 20 °C (68 °F)
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

Relative vapor density	4.90 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity
No data available

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .
Contains the following stabilizer(s):
Copper(bulk) (%)

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
no information available

10.5 Incompatible materials
Strong oxidizing agents, Strong bases, Oxygen

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 79.84 mg/kg
(OECD Test Guideline 401)
Remarks: The value is given in analogy to the following substances: iodomethane
LC50 Inhalation - Rat - male and female - 4 h - 4.076 mg/l - vapor

(US-EPA)
Remarks: The value is given in analogy to the following substances: iodomethane
Acute toxicity estimate Dermal - 1,100.1 mg/kg
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: iodomethane

Skin corrosion/irritation
Skin - Rabbit
Result: Irritations - 4 h
(OECD Test Guideline 404)
Remarks: The value is given in analogy to the following substances: iodomethane
Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation
(OECD Test Guideline 405)
Remarks: The value is given in analogy to the following substances: iodomethane

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative
(OECD Test Guideline 406)
Remarks: The value is given in analogy to the following substances: iodomethane

Germ cell mutagenicity
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: US-EPA
Result: negative
Remarks: The value is given in analogy to the following substances: iodomethaneTest Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: US-EPA
Result: negative
Remarks: The value is given in analogy to the following substances: iodomethaneTest Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: US-EPA
Result: positive

Remarks: The value is given in analogy to the following substances: iodomethane
Test Type: In vivo micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal injection
Method: US-EPA
Result: negative
Remarks: The value is given in analogy to the following substances: iodomethane

Carcinogenicity
Suspected of causing cancer.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation. - Respiratory system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: iodomethane

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 5 mg/kg
Remarks: Subchronic toxicity
The value is given in analogy to the following substances: iodomethane

Repeated dose toxicity - Rat - male and female - Dermal - 28 d - NOAEL (No observed adverse effect level) - 30 mg/kg
Remarks: Subacute toxicity
The value is given in analogy to the following substances: iodomethane

Nausea, Dizziness, Headache, Blurred vision, Weakness, Drowsiness, Ataxia., Confusion., Convulsions, narcosis, Pulmonary edema. Effects may be delayed., Symptoms of systemic copper poisoning may include: capillary damage, headache, cold sweat, weak pulse, and kidney and liver damage, central nervous system excitation followed by depression, jaundice, convulsions, paralysis, and coma. Death may occur from shock or renal failure. Chronic copper poisoning is typified by hepatic cirrhosis, brain damage and demyelination, kidney defects, and copper deposition in the cornea as exemplified by humans with Wilson's disease. It has also been reported that copper poisoning has lead to hemolytic anemia and accelerates arteriosclerosis.

Nausea, Dizziness, Headache, Blurred vision, Weakness, Drowsiness, Ataxia., Confusion., Convulsions, narcosis, Pulmonary edema. Effects may be delayed.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Liver - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 1.4 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: iodomethane
	semi-static test NOEC - Oncorhynchus mykiss (rainbow trout) - 0.62 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: iodomethane
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.57 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: iodomethane
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (algae) - 1.69 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: iodomethane
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 0.16 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances: iodomethane

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 0 % - Not biodegradable (OECD Test Guideline 301F) Remarks: The value is given in analogy to the following substances: iodomethane

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 2644 Class: 6.1I Packing group: I
Proper shipping name: Methyl iodide
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: Hazard Zone B

IMDG
UN number: 2644 Class: 6.1 Packing group: I EMS-No: F-A, S-A
Proper shipping name: METHYL IODIDE

IATA
UN number: 2644 Class: 6.1
Proper shipping name: Methyl iodide
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
iodomethane-d_3	865-50-9	100	100

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

iodomethane-d_3	865-50-9	>= 90 - <= 100 %

US State Regulations

Massachusetts Right To Know

iodomethane-d_3 865-50-9

Pennsylvania Right To Know

iodomethane-d_3 865-50-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

California Prop. 65

WARNING: This product can expose you to chemicals including iodomethane-d_3, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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