

SAFETY DATA SHEET

Version 6.10
Revision Date 08/08/2025
Print Date 08/09/2025

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Iodomethane-¹³C
Product Number : 277185
Brand : Aldrich
CAS-No. : 4227-95-6

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute toxicity (Oral) : Category 3

Acute toxicity (Inhalation) : Category 3

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Acute toxicity (Dermal) : Category 4
Skin irritation : Category 2
Carcinogenicity : Category 2
Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal Word : Danger

Hazard Statements : H301 + H331 Toxic if swallowed or if inhaled.
H312 Harmful in contact with skin.
H315 Causes skin irritation.
H335 May cause respiratory irritation.
H351 Suspected of causing cancer.

Precautionary statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing mist or vapours.
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.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

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.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Iodomethane-13C	4227-95-6*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves. Show this 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.

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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides Hydrogen iodide
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.
- Further information on storage conditions : Tightly closed.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 6.1B, Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
- Recommended storage temperature : 36 - 46 °F / 2 - 8 °C
- Further information on storage stability : Light sensitive.
Moisture sensitive.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Iodomethane-13C	4227-95-6	TWA	2 ppm	ACGIH
		TWA	2 ppm 10 mg/m ³	NIOSH REL

		TWA	5 ppm 28 mg/m ³	OSHA Z-1
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Engineering measures : No data available

Personal protective equipment

Respiratory protection : 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.

Recommended Filter type: : Filter type AX

The entrepreneur 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.

Hand protection

Remarks : required

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

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : colourless

Odor : No data available

Odor Threshold : No data available
pH : No data available

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Melting point/ range	: -87.7 °F / -66.5 °C Method: lit.
Boiling point/boiling range	: 108 °F / 42 °C Method: lit.
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: The product is not flammable.
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: 1,518.5 hPa (131 °F / 55 °C) 437.7 hPa (68 °F / 20 °C)
Relative vapour density	: 4.93 (Air = 1.0)
Relative density	: No data available
Density	: 2.29 g/cm ³ (77 °F / 25 °C)
Solubility(ies) Water solubility	: soluble (68 °F / 20 °C)
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available

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Oxidizing properties : No data available

Molecular weight : 142.92 g/mol

Particle characteristics
Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : No data available

Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .

Contains the following stabiliser(s): : Copper(bulk) (≥ 0 - < 10 %)

Possibility of hazardous reactions : No data available

Conditions to avoid : Avoid moisture.
no information available

Incompatible materials : Strong oxidizing agents
Strong bases

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 - vapour

(US-EPA)

Remarks: The value is given in analogy to the following substances: iodomethane
Acute toxicity estimate Dermal - 1,100.1 mg/kg
(Expert judgement)

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

Maximisation 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 component 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 component 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 - 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 - 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.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Iodomethane-13C:

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 1.4 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 203
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: iodomethane

NOEC (Oncorhynchus mykiss (rainbow trout)): 0.62 mg/l

End point: mortality
 Exposure time: 96 h
 Test Type: semi-static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 203
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: iodomethane

- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 0.57 mg/l
 End point: Immobilization
 Exposure time: 48 h
 Test Type: static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 202
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: iodomethane
- Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (algae)): 1.69 mg/l
 Exposure time: 72 h
 Test Type: static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 201
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: iodomethane
- M-Factor (Acute aquatic toxicity) : 1
- Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 0.16 mg/l
 End point: reproduction rate
 Exposure time: 21 d
 Test Type: semi-static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 211
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: iodomethane

Persistence and degradability

Components:

Iodomethane-13C:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Not biodegradable
Biodegradation: 0 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: iodomethane

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

Product:

Additional ecological information : An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

Not permitted for transport

IMDG-Code

UN number : UN 2644
Proper shipping name : METHYL IODIDE

Class : 6.1
Packing group : I

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Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2644
Proper shipping name : Methyl iodide

Class : 6.1
Packing group : I
Labels : Division 6.1 - Poison inhalation hazard
ERG Code : 151
Marine pollutant : no

Poison Inhalation Hazard : Hazard Zone B

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Iodomethane-13C	4227-95-6	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- 4227-95-6 >= 90 - <= 100 %
13C

US State Regulations

Massachusetts Right To Know

Iodomethane-13C

4227-95-6

Pennsylvania Right To Know

Iodomethane-13C

4227-95-6

Copper(bulk)

7440-50-8

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-13C, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

The components 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

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL : USA. NIOSH Recommended Exposure Limits
OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA : 8-hour, time-weighted average
NIOSH REL / TWA : Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
OSHA Z-1 / TWA : 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA -

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International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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.

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Revision Date : 08/08/2025

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