

SAFETY DATA SHEET

Version 8.6 Revision Date 09/06/2024 Print Date 12/21/2024

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

1.1 Product identifiers

Product name : Iodoethane-1,1-d₂

Product Number : 486736 Brand : Aldrich CAS-No. : 3652-82-2

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)

Flammable liquids (Category 4), H227 Acute toxicity, Oral (Category 4), H302 Skin irritation (Category 2), H315 Eye irritation (Category 2A), H319

Aldrich - 486736

Page 1 of 12



Respiratory sensitization (Category 1), H334

Skin sensitization (Category 1), H317

Germ cell mutagenicity (Category 2), H341

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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
nazaru	Statements

H227	Combustible liquid.	
H302	Harmful if swallowed.	
H315	Causes skin irritation.	

H317 May cause an allergic skin reaction. H319 Causes serious eye irritation.

H334 May cause allergy or asthma symptoms or breathing difficulties

if inhaled.

H335 May cause respiratory irritation. H341 Suspected of causing genetic defects.

Precautionary Statements

P201 Obtain special instructions before us
--

P202 Do not handle until all safety precautions have been read and

understood.

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No

smoking.

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.

P272 Contaminated work clothing must not be allowed out of the

workplace.

P280 Wear protective gloves/ protective clothing/ eye protection/ face

protection.

P285 In case of inadequate ventilation wear respiratory protection.

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel

unwell. Rinse mouth.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue

rinsing.

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.

P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/

doctor

P362 Take off contaminated clothing and wash before reuse.

Aldrich - 486736

MILLIPORE

Page 2 of 12

P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam 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 an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Ethyl-1,1-d2 iodide

Formula : $C_2D_2H_3I$ Molecular weight : 157.98 g/mol CAS-No. : 3652-82-2 EC-No. : 623-327-6

Component	Classification	Concentration
1-Iodoethane-1,1-d2		
	Flam. Liq. 4; Acute Tox. 4;	<= 100 %
	Skin Irrit. 2; Eye Irrit. 2A;	
	Resp. Sens. 1; Skin Sens.	
	1; Muta. 2; STOT SE 3;	
	H227, H302, H315, H319,	
	H334, H317, H341, H335	

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. Call in physician.

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.

Aldrich - 486736



Page 3 of 12

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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.

Aldrich - 486736

Page 4 of 12



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.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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 locked up or in an area accessible only to qualified or authorized persons.

Storage stabilityRecommended storage temperature

2 - 8 °C

Storage class

Storage class (TRGS 510): 10: Combustible liquids

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

Contains no substances with occupational exposure limit values.

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

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other

Aldrich - 486736

Page 5 of 12



substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Full contact Material: Viton®

Minimum layer thickness: 0.7 mm Break through time: 480 min

Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Splash contact Material: Viton®

Minimum layer thickness: 0.7 mm Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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, clear
b) Odor No data available
c) Odor Threshold No data available
d) pH No data available

e) Melting point/ range: -108 °C (-162 °F) - lit.

point/freezing point

f) Initial boiling point 69 - 73 °C 156 - 163 °F - lit. and boiling range

g) Flash point 72 °C (162 °F) - closed cup

Aldrich - 486736 Page 6 of 12

Millipore Sigma h) Evaporation rate No data availablei) Flammability (solid, No data available gas)

j) Upper/lower No data available flammability or explosive limits

k) Vapor pressure No data available l) Vapor density 5.38 - (Air = 1.0)

m) Density 1.974 g/mL at 25 °C (77 °F)

Relative density

No data available

No data available

No data available

No data available

n-octanol/water

p) Autoignition No data available temperature

q) Decomposition No data available temperature

r) Viscosity No data available

s) Explosive properties Not classified as explosive.

t) Oxidizing properties none

9.2 Other safety information

Relative vapor 5.38 - (Air = 1.0) density

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) . May decompose on exposure to moist air or water.

10.3 Possibility of hazardous reactions

Risk of explosion with:

Fluorine

sodium

Exothermic reaction with:

phosphorus

ethanol

Violent reactions possible with:

Aldrich - 486736



Metals strong alkalis Strong oxidizing agents magnesium Mercury

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data available

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 - 330 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: iodoethane

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of

respiratory tract

Dermal: No data available

Skin corrosion/irritation

Remarks: Causes skin irritation.

The value is given in analogy to the following substances: iodoethane

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.

The value is given in analogy to the following substances: iodoethane

Respiratory or skin sensitization

May cause allergic respiratory and skin reactions The value is given in analogy to the following substances:

Germ cell mutagenicity

Suspected of causing genetic defects.

Carcinogenicity

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

Aldrich - 486736

4illiPDRE

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory system

Remarks: The value is given in analogy to the following substances: iodoethane

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

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

narcosis, Cough, Shortness of breath, irritant effects

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

Absorption may result in damage of the following:

Central nervous system

Liver

Kidney

Lungs

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

 $\label{pbt} PBT/vPvB \ assessment \ not \ available \ as \ chemical \ safety \ assessment \ not \ required/not \ conducted$

12.6 Endocrine disrupting properties

No data available

Aldrich - 486736

Page 9 of 12



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)

NA-Number: 1993 Class: NONE Packing group: III

Proper shipping name: Combustible liquid, n.o.s. (1-Iodoethane-1,1-d2)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

Not dangerous goods

IATA

Not dangerous goods

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

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 : Fire Hazard

Hazards Acute Health Hazard Chronic Health Hazard

Aldrich - 486736 Page 10 of 12

SARA 313

: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

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

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.

Aldrich - 486736

....

Page 11 of 12

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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.

Version: 8.6 Revision Date: 09/06/2024 Print Date: 12/21/2024

Aldrich - 486736

