

## SAFETY DATA SHEET

Version 6.12  
Revision Date 09/08/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1,2-Dichlorobenzene-d<sub>4</sub>

Product Number : 331511  
Brand : Aldrich  
CAS-No. : 2199-69-1

**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  
Acute toxicity, Inhalation (Category 4), H332  
Skin irritation (Category 2), H315

Aldrich - 331511

Page 1 of 13

Eye irritation (Category 2A), H319  
 Skin sensitization (Sub-category 1B), H317  
 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

Warning

Hazard Statements

H227	Combustible liquid.
H302 + H332	Harmful if swallowed or if inhaled.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H410	Very toxic to aquatic life with long lasting effects.

Precautionary Statements

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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face 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.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
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	: Tetradeutero-1,2-dichlorobenzene
Formula	: C <sub>6</sub> D <sub>4</sub> Cl <sub>2</sub>
Molecular weight	: 151.03 g/mol
CAS-No.	: 2199-69-1
EC-No.	: 218-606-0

Component	Classification	Concentration
<b>1,2-dichlorobenzene-d<sub>4</sub></b>		
	Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Skin Sens. 1B; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H227, H302, H332, H315, H319, H317, H335, H400, H410	<= 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

Show this material safety data sheet to the doctor in attendance.

##### If inhaled

After inhalation: fresh air.

##### 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

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

Aldrich - 331511

Page 3 of 13

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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 chloride gas

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.

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## 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 with liquid-absorbent material (e.g. Chemisorb® ). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### **Advice on safe handling**

Aldrich - 331511

Page 4 of 13

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 in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Light sensitive. hygroscopic Store under inert gas.

### Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

## 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
1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1	TWA	25 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		
		C	50 ppm 300 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		C	50 ppm 300 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	50 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

		PEL	25 ppm 150 mg/m <sup>3</sup>	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

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](http://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](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

#### Body Protection

protective clothing

#### Respiratory protection

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

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.

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.

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### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid, clear Color: colorless, light yellow
b) Odor	characteristic
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: -18 - -17 °C (-0.40 - 1 °F)
f) Initial boiling point and boiling range	178 - 180 °C 352 - 356 °F - lit.
g) Flash point	66.0 °C (150.8 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 12 %(V) Lower explosion limit: 2.2 %(V)
k) Vapor pressure	1.33 hPa at 20 °C (68 °F)
l) Vapor density	5.1
m) Density	1.341 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	0.13 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: 3.43 at 25 °C (77 °F) - Bioaccumulation is not expected.
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	5.1
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## 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) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Alkali metals  
Alkaline earth metals  
Strong oxidizing agents  
Halogenated hydrocarbon  
Aluminum  
Light metals

### 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

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 2,000 mg/kg

(OECD Test Guideline 401)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

The value is given in analogy to the following substances: 1,2-Dichlorobenzene

Acute toxicity estimate Inhalation - 4 h - 11.1 mg/l - vapor

(Expert judgment)

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene

LD50 Dermal - Rabbit - > 10,000 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: 1,2-Dichlorobenzene

#### Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene



**Serious eye damage/eye irritation**

Remarks: Causes serious eye irritation.

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: 1,2-Dichlorobenzene

**Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene

**Germ cell mutagenicity**

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: 1,2-

DichlorobenzeneTest Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: 1,2-

DichlorobenzeneTest Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene

Test Type: In vivo micronucleus test

Species: Rat

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene

Test Type: comet assay

Species: Rat

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 489

Result: negative

Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene

**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

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation. - Respiratory Tract

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: 1,2-Dichlorobenzene

**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 Days - NOAEL (No observed adverse effect level) - 60 mg/kg - LOAEL (Lowest observed adverse effect level) - 125 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: 1,2-Dichlorobenzene

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

Stomach - Irregularities - Based on Human Evidence

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish	flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 1.58 mg/l - 96 h Remarks: (ECHA) The value is given in analogy to the following substances: 1,2-Dichlorobenzene
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Ceriodaphnia dubia (water flea) - 0.66 mg/l - 48 h (US-EPA) Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene
Toxicity to algae	ErC50 - Pseudokirchneriella subcapitata (green algae) - 2.2 mg/l - 96 h (US-EPA) Remarks: The value is given in analogy to the following substances: 1,2-Dichlorobenzene
Toxicity to daphnia and other aquatic	semi-static test EC50 - Daphnia magna (Water flea) - 0.55 mg/l - 14 d

Aldrich - 331511

Page 10 of 13

invertebrates(Chronic toxicity)      Remarks: (ECHA)  
The value is given in analogy to the following substances: 1,2-Dichlorobenzene

## **12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: 0 % - Not readily biodegradable.  
(OECD Test Guideline 301C)  
Remarks: The value is given in analogy to the following substances:  
1,2-Dichlorobenzene

## **12.3 Bioaccumulative potential**

Bioaccumulation      Cyprinus carpio (Carp) - 56 d  
at 25 °C - 0.01 mg/l(1,2-dichlorobenzene-d4)  
  
Bioconcentration factor (BCF): 90 - 260  
(OECD Test Guideline 305C)  
  
Remarks: The value is given in analogy to the following substances:  
1,2-Dichlorobenzene

## **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

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## **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.

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**SECTION 14: Transport information****DOT (US)**

UN number: 1591 Class: 6.1 Packing group: III  
Proper shipping name: o-Dichlorobenzene  
Reportable Quantity (RQ): 100 lbs  
Reportable Quantity (RQ): 10 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1591 Class: 6.1 Packing group: III EMS-No: F-A, S-A  
Proper shipping name: o-DICHLOROBENZENE  
Marine pollutant : yes

**IATA**

UN number: 1591 Class: 6.1 Packing group: III  
Proper shipping name: o-Dichlorobenzene

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1	100	100
1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1		100
1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1	10	10 (F002)

**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** : Fire Hazard  
Acute Health Hazard

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

1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1	>= 90 - <= 100 %
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**US State Regulations****Massachusetts Right To Know**

1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1
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**Pennsylvania Right To Know**

1,2-dichlorobenzene-d <sub>4</sub>	2199-69-1
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**Maine Chemicals of High Concern**

Aldrich - 331511

Page 12 of 13

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.

The following substance(s) is/are subject to TSCA 12(b) export notification requirements:  
1,2-dichlorobenzene-d<sub>4</sub> 2199-69-1

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**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](http://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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Details in analogy to the undeuterated compound.

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