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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**Product name : Chlorobenzene-d<sub>5</sub>

Product Number : 176605

Brand : Aldrich

CAS-No. : 3114-55-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Acute toxicity, Inhalation (Category 4), H332

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

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 statement(s)

H226 : Flammable liquid and vapour.

H332 : Harmful if inhaled.

H411 : Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

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

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.

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/ physician if you feel unwell.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Chemical characterization : Isotopically labeled  
 Synonyms : Pentadeuteriochlorobenzene

Formula : C<sub>6</sub>D<sub>5</sub>Cl  
 Molecular weight : 117.59 g/mol  
 CAS-No. : 3114-55-4  
 EC-No. : 221-482-0

#### Hazardous components

Component	Classification	Concentration
<b>Chlorobenzene-D5</b>		
	Flam. Liq. 3; Acute Tox. 4; Aquatic Acute 2; Aquatic Chronic 2; H226, H332, H411	<= 100 %

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

### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

##### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

##### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

##### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

##### In case of eye contact

Flush eyes with water as a precaution.

##### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Handle and store under inert gas.

### 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
	Remarks	See Appendix D - Substances with No Established RELs		
Chlorobenzene-D5	3114-55-4	TWA	75.000000 ppm 350.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		

		PEL	10 ppm 46 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
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## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |   |
|---|---|
| a) Appearance                                   | Form: liquid, clear<br>Colour: colourless                           |
| b) Odour  | No data available   |
| c) Odour Threshold                              | No data available   |
| d) pH   | No data available   |
| e) Melting point/freezing point                 | No data available   |
| f) Initial boiling point and boiling range      | 130 - 130.5 °C (266 - 266.9 °F) - lit.                              |
| g) Flash point                                  | 24.0 °C (75.2 °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: 7.1 %(V)<br>Lower explosion limit: 1.3 %(V)  |
| k) Vapour pressure                              | No data available   |
| l) Vapour density                               | No data available   |
| m) Relative density                             | 1.157 g/mL at 25 °C (77 °F)1.157 g/cm <sup>3</sup> at 25 °C (77 °F) |
| n) Water solubility                             | No data available   |

- |   |                   |
|---|-------------------|
| o) Partition coefficient: n-octanol/water | log Pow: 2.710    |
| p) Auto-ignition temperature              | No data available |
| q) Decomposition temperature              | No data available |
| r) Viscosity                              | No data available |
| s) Explosive properties                   | No data available |
| t) Oxidizing properties                   | No data available |

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

- 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

Nausea, Dizziness, Headache, Liver injury may occur., Kidney injury may occur.

Testes. -

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**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**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life with long lasting effects.

No data available

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**13. DISPOSAL CONSIDERATIONS**

**13.1 Waste treatment methods**

**Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION**

**DOT (US)**

UN number: 1134

Class: 3

Packing group: III

Proper shipping name: Chlorobenzene

Reportable Quantity (RQ): 100 lbs

Poison Inhalation Hazard: No

**IMDG**

UN number: 1134      Class: 3      Packing group: III      EMS-No: F-E, S-D  
Proper shipping name: CHLOROBENZENE  
Marine pollutant:yes

**IATA**

UN number: 1134      Class: 3      Packing group: III  
Proper shipping name: Chlorobenzene

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**15. REGULATORY INFORMATION**

**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

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

	CAS-No.	Revision Date
Chlorobenzene-D5	3114-55-4	2007-07-01

**SARA 311/312 Hazards**

Fire Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
Chlorobenzene-D5	3114-55-4	2007-07-01

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Chlorobenzene-D5	3114-55-4	2007-07-01

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
Chlorobenzene-D5	3114-55-4	2007-07-01

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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**16. OTHER INFORMATION**

**Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H332	Harmful if inhaled.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

**HMIS Rating**

Health hazard:	1
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

**NFPA Rating**

Health hazard:	1
Fire Hazard:	3
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 4.8

Revision Date: 09/26/2016

Print Date: 11/09/2018