

## SAFETY DATA SHEET

Version 8.9  
Revision Date 03/02/2024  
Print Date 05/26/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Chlorobenzene for synthesis

Product Number : 8.01791  
Catalogue No. : 801791  
Brand : Millipore  
Index-No. : 602-033-00-1  
CAS-No. : 108-90-7

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

Identified uses : Chemical for synthesis  
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 3), H226  
Acute toxicity, Inhalation (Category 4), H332  
Skin irritation (Category 2), H315

Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (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 Statements

H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H332	Harmful if inhaled.
H411	Toxic to aquatic life with long lasting effects.

Precautionary Statements

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 mist or vapors.
P264	Wash skin thoroughly after handling.
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): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P332 + P313	If skin irritation occurs: 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 + 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

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### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Formula	:	C6H5Cl
Molecular weight	:	112.56 g/mol
CAS-No.	:	108-90-7
EC-No.	:	203-628-5

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**MILLIPORE  
SIGMA**

Index-No. : 602-033-00-1

Component	Classification	Concentration
<b>chlorobenzene</b>		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Aquatic Acute 2; Aquatic Chronic 2; H226, H332, H315, H401, H411	<= 100 %

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

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## 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. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

#### In case of skin contact

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

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

### 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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## 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.

Fire may cause evolution of:

Hydrogen chloride gas, Phosgene

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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. Risk of explosion.

### 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. Chemizorb® ). 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

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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

### Storage class

Storage class (TRGS 510): 3: Flammable 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

Component	CAS-No.	Value	Control parameters	Basis
chlorobenzene	108-90-7	TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans		
		TWA	75 ppm 350 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	10 ppm 46 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
chlorobenzene	108-90-7	4-Chlorocatechol	100mg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			
		p-Chlorophenol	20mg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift at end of workweek			

### 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: 10 min

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

### Body Protection

Flame retardant antistatic 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. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |                                  |
|---------------|----------------------------------|
| a) Appearance | Form: liquid<br>Color: colorless |
| b) Odor       | weak                             |

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c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	132 °C 270 °F at 1,013 hPa
g) Flash point	27 °C (81 °F) - DIN 51755 Part 1
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 11 %(V) Lower explosion limit: 1.3 %(V)
k) Vapor pressure	12.05 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	1.11 g/cm <sup>3</sup> at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	0.207 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: 2.84 at 20 °C (68 °F) - - Bioaccumulation is not expected., (ECHA)
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

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Exothermic reaction with:  
Alkali metals

Alkaline earth metals  
Oxidizing agents  
dimethyl sulfoxide  
Nitric acid  
Risk of explosion with:  
sodium  
in finely distributed form.  
with  
sodium

#### **10.4 Conditions to avoid**

Heating.

#### **10.5 Incompatible materials**

rubber

#### **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)

LC50 Inhalation - Rat - male - 4 h - 15.57 mg/l - vapor

(OECD Test Guideline 403)

Dermal: No data available

##### **Skin corrosion/irritation**

Skin - Rabbit

Result: Skin irritation - 4 h

(OECD Test Guideline 404)

##### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

##### **Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

##### **Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test):



Test system: Chinese hamster lung cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative  
Test 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

### **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**

No data available

### **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.

Systemic effects:

CNS disorders  
tachycardia  
drop in blood pressure  
agitation, spasms  
ataxia (impaired locomotor coordination)  
narcosis  
Headache

Damage to:

Liver  
Kidney

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	static test LC50 - Lepomis macrochirus (Bluegill sunfish) - 4.5 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 26 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC10 - Desmodesmus subspicatus (green algae) - 5.8 mg/l - 72 h (OECD Test Guideline 201) static test ErC50 - Desmodesmus subspicatus (green algae) - 11.4 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 140 mg/l - 30 min (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	semi-static test NOEC - Danio rerio (zebra fish) - 4.8 mg/l - 28 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - Daphnia magna (Water flea) - 0.72 mg/l - 21 d (OECD Test Guideline 211)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 15 % - Not readily biodegradable. (OECD Test Guideline 301F) aerobic - Exposure time 28 d Result: 0 % - Not readily biodegradable. (OECD Test Guideline 301C)
Theoretical oxygen demand	2,060 mg/g Remarks: (Lit.)
Ratio BOD/ThBOD	1.5 % Remarks: (Lit.)

### 12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 49 d at 25 °C(chlorobenzene)  Bioconcentration factor (BCF): 3.9 - 23 (OECD Test Guideline 305C)
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### 12.4 Mobility in soil

No data available

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## 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

Discharge into the environment must be avoided.

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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: 1134 Class: 3 Packing group: III  
Proper shipping name: Chlorobenzene  
Reportable Quantity (RQ): 100 lbs  
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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## SECTION 15: Regulatory information

### SARA 302 Components

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

### SARA 313 Components

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

chlorobenzene	CAS-No. 108-90-7	Revision Date 2007-07-01
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**Reportable Quantity** : D021 lbs

**Massachusetts Right To Know Components**

chlorobenzene	CAS-No. 108-90-7	Revision Date 2007-07-01
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**Pennsylvania Right To Know Components**

chlorobenzene	CAS-No. 108-90-7	Revision Date 2007-07-01
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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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Version: 8.9

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