

# SAFETY DATA SHEET

Version 6.17 Revision Date 07/04/2025 Print Date 07/05/2025

#### **SECTION 1. IDENTIFICATION**

#### 1.1 Product identifiers

Product name : Benzyl chloroformate (stabilised) for

synthesis

Product Number : 8.14688
Catalogue No. : 814688
Brand : Millipore
Index-No. : 607-064-00-4
CAS-No. : 501-53-1

#### 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 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)

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Flammable liquids : Category 4

Skin corrosion : Sub-category 1B

Serious eye damage : Category 1

Skin sensitisation : Category 1

Carcinogenicity Category 1B

Short-term (acute) aquatic hazard

Category 1

Long-term (chronic)

aquatic hazard

: Category 1

### Other hazards

None known.

#### **GHS label elements**

Hazard pictograms









Signal Word Danger

Hazard Statements : H227 Combustible liquid.

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction. H335 May cause respiratory irritation.

H350 May cause cancer.

H410 Very toxic to aquatic life with long lasting effects.

Supplemental Hazard

Statements

: Corrosive to the respiratory tract.

Precautionary statements:

## **Prevention:**

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have

been read and understood.

P210 Keep away from heat, hot surfaces, sparks, open

flames and other ignition sources. No smoking.

P261 Avoid breathing mist or vapours. P264 Wash skin thoroughly after handling.

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, protective clothing, eye

protection and face protection.

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### Response:

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor. P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor. P308 + P313 IF exposed or concerned: Get medical advice/ attention.

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

P362 + P364 Take off contaminated clothing and wash it before reuse.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

### 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
Benzyl chloroformate	501-53-1*	>= 80 - <= 100	TSC
Benzyl chloride	100-44-7*	>= 0.1 - <= 1	TSC

<sup>\*</sup> Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

#### **SECTION 4. FIRST AID MEASURES**

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General advice : First aiders need to protect themselves.

Show this 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.

Call a physician immediately.

In case of eye contact : After eye contact: rinse out with plenty of water.

Immediately call in ophthalmologist.

Remove contact lenses.

If swallowed : After swallowing: make victim drink water (two

glasses at most), avoid vomiting (risk of perforation).

Call a physician immediately. Do not attempt to neutralise.

Most important symptoms and effects.

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 (CO2)

Dry powder

Unsuitable extinguishing

media

: For this substance/mixture no limitations of

extinguishing agents are given.

Specific hazards during

fire fighting

: Combustible.

Caution! in contact with water product releases:

hydrochloric acid

Fire may cause evolution of:

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Hydrogen chloride gas

Vapours 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.

Hazardous combustion products

: Carbon oxides

Hydrogen chloride gas

Specific extinguishing methods

: No data available

Further information

: Remove container from danger zone and cool with

water.

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.

Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency

procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

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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 protection against fire and explosion Keep away from open flames, hot surfaces and

sources of ignition.

Take precautionary measures against static discharge.

Advice on safe handling

Keep workplace dry. Do not allow product to come

into contact with water.

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.

: 6.1C, Combustible, acute toxic Cat.3 / toxic Storage class

compounds or compounds which causing chronic

effects

Recommended storage

temperature

: Recommended storage temperature see product label.

Further information on

storage stability

: Recommended storage temperature see product label.

# SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

•	•			
Components	CAS-No.	Value type	Control	Basis
		(Form of	parameters /	
		exposure)	Permissible	
			concentration	
Benzyl chloride	100-44-7	TWA	1 ppm	ACGIH
		С	1 ppm	NIOSH REL
			5 mg/m3	

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TWA 1 ppm OSHA Z-1 5 mg/m3

**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 ABEK

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.

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).

Tightly fitting safety goggles

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 : stinging

Odor Threshold : No data available

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рΗ : No data available

Melting point : -0.40 °F / -18 °C

: 217 °F / 103 °C (25 hPa)

Flash point : 198 °F / 92 °C

Method: c.c., closed cup

: No data available Evaporation rate

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

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 hPa (68 °F / 20 °C)

Relative vapour density : 5.89

Relative density : No data available

Density : 1.21 g/cm3 (68 °F / 20 °C)

Solubility(ies)

Water solubility : (rigorous decomposition) (68 °F / 20 °C)

Partition coefficient: n-

octanol/water

: No data available

Autoignition temperature : 1094 °F / 590 °C

Decomposition

temperature

: No data available

Viscosity

: 2.36 mPa.s (68 °F / 20 °C) Viscosity, dynamic

Viscosity, kinematic : No data available

: No data available Flow time

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Explosive properties : Not classified as explosive.

Oxidizing properties : none

Molecular weight : 170.59 g/mol

Particle characteristics

Particle size : No data available

#### **SECTION 10. STABILITY AND REACTIVITY**

Reactivity : has a corrosive effect

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point

is to be rated as critical.

Chemical stability : sensitive to moisture

The product is chemically stable under standard

ambient conditions (room temperature) .

Contains the following

stabiliser(s):

: sodium carbonate (0.1 %)

Possibility of hazardous

reactions

: can decompose violently in contact with:

Amines

Conditions to avoid : Moisture.

Strong heating.

Incompatible materials : No data available

products

Hazardous decomposition : In the event of fire: see section 5

#### **SECTION 11. TOXICOLOGICAL INFORMATION**

### 11.1 Information on toxicological effects

### **Acute toxicity**

LD50 Oral - Rat - 3,000 mg/kg LD50 Oral - Rat - 3,000 mg/kg

Remarks: (RTECS)

Acute toxicity estimate Inhalation - 4 h - > 200 mg/l - vapour(Calculation method)

Dermal: No data available Skin corrosion/irritation

No data available

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# Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

## Respiratory or skin sensitization

No data available

# Germ cell mutagenicity

No data available

### Carcinogenicity

IARC: 2A - Group 2A: Probably carcinogenic to humans (Benzyl chloride)

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

No data available

# Specific target organ toxicity - repeated exposure

No data available

## **Aspiration hazard**

No data available

### 11.2 Additional Information

Nausea, Shock.

### **SECTION 12. ECOLOGICAL INFORMATION**

## **Ecotoxicity**

## **Product:**

# **Ecotoxicology Assessment**

Acute aquatic toxicity : Very toxic to aquatic life.

### **Components:**

#### **Benzyl chloroformate:**

Toxicity to fish : LC50 (Danio rerio (zebra fish)): > 4.64 - < 10 mg/l

Exposure time: 96 h Remarks: (Hommel)

# **Ecotoxicology Assessment**

Acute aquatic toxicity : Very toxic to aquatic life.

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

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**Benzyl chloride:** 

Toxicity to fish : LC50 (Danio rerio (zebra fish)): 4 mg/l

Exposure time: 96 h Test Type: static test

Method: OECD Test Guideline 203

Toxicity to daphnia and

other aquatic invertebrates

: EC50 (Daphnia magna (Water flea)): 6.1 mg/l

End point: Immobilization Exposure time: 48 h Test Type: static test

Method: OECD Test Guideline 202

GLP: yes

# Persistence and degradability

### **Components:**

# Benzyl chloride:

Biodegradability : aerobic

Inoculum: activated sludge Concentration: 100 mg/l Result: Readily biodegradable.

Biodegradation: 71 % Exposure time: 14 d

Method: OECD Test Guideline 301C

Stability in water : Test substance: Water

Remarks: Rapid degradation.

## **Bioaccumulative potential**

### **Components:**

# Benzyl chloride:

Partition coefficient: n- : log Pow: 2.3

octanol/water Method: (experimental)
Remarks: (IUCLID)

Bioaccumulation is not expected.

# Mobility in soil

No data available

# Other adverse effects

#### **Product:**

Ozone-Depletion Potential: Regulation: 40 CFR Protection of Environment; Part

82 Protection of Stratospheric Ozone - CAA Section

602 Class I Substances

Remarks: 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

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82, Subpt. A, App.A + B).

Additional ecological

information

: The following may develop after reaction of the

product with water:

hydrochloric acid

After hydrolysis acid effect on fish and plankton.

Harmful effect due to pH shift.

Forms corrosive mixtures with water even if diluted.

Discharge into the environment must be avoided.

### **Components:**

## **Benzyl chloride:**

Additional ecological information

: Discharge into the environment must be avoided.

#### **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

UN/ID No. : UN 1739

Proper shipping name : Benzyl chloroformate

Class : 8 Packing group : I

Labels : Class 8 - Corrosive substances

Packing instruction (cargo: 854

aircraft)

Packing instruction : Not permitted for transport

(passenger aircraft)

IMDG-Code

UN number : UN 1739

Proper shipping name : BENZYL CHLOROFORMATE

Class : 8 Packing group : I

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Labels : 8

EmS Code : F-A, <u>S-B</u> Marine pollutant : yes

# Transport in bulk according to IMO instruments

Not applicable for product as supplied.

# **National Regulations**

#### 49 CFR Road

UN/ID/NA number : UN 1739

Proper shipping name : Benzyl chloroformate

Class : 8 Packing group : I

Labels : Class 8 - Corrosive substances

ERG Code : 137 Marine pollutant : yes

Poison Inhalation Hazard : No

# **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**

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

#### SARA 304 Extremely Hazardous Substances Reportable Quantity

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

#### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

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).

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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

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

Benzyl chloride 100-44-7  $\Rightarrow 0.1 - < 1 \%$ 

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

Benzyl chloride 100-44-7 >= 0.1 - < 1 %

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**

Benzyl chloride 100-44-7

Pennsylvania Right To Know

Benzyl chloride 100-44-7

# **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 Benzyl chloride, 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 : All substances listed as active on the 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

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: Ceiling value not be exceeded at any time. NIOSH REL / C

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 Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA -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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO -International Organisation for Standardization; 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 - Organization 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-Decomposition Temperature; SARA Superfund Amendments 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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