

# **SAFETY DATA SHEET**

Version 6.5 Revision Date 09/09/2021 Print Date 09/25/2021

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

#### 1.1 Product identifiers

Product name : 4-Nitrobenzoyl chloride

Product Number : 112208
Brand : Aldrich
CAS-No. : 122-04-3

# 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 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)

Skin corrosion (Category 1B), H314 Serious eye damage (Category 1), H318

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 statement(s)

H314 Causes severe skin burns and eye damage.

H318 Causes serious eye damage.

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Precautionary statement(s)	
P260	Do not breathe dusts or mists.
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Immediately call a POISON CENTER or doctor/ physician.
P305 + P351 + P338 +	IF IN EYES: Rinse cautiously with water for several minutes.
P310	Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363	Wash contaminated clothing before reuse.
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 Lachrymator.

# **SECTION 3: Composition/information on ingredients**

#### 3.1 Substances

Formula :  $C_7H_4CINO_3$ Molecular weight : 185.56 g/mol CAS-No. : 122-04-3EC-No. : 204-517-4

Component	Classification	Concentration
4-nitrobenzoyl chloride		
	Met. Corr. 1; Skin Corr. 1B; Eye Dam. 1; H290,	<= 100 %
	H314, H318	

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**

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

#### If inhaled

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

#### In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.



## In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

#### 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

# **SECTION 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

Carbon oxides Nitrogen oxides (NOx) Hydrogen chloride gas Combustible.

# 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

#### SECTION 6: Accidental release measures

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. 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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### 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

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# Avoid formation of dust and aerosols. Advice on safe handling

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

# Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

#### **Hygiene measures**

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

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.

Moisture sensitive.

## Storage class

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

# 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**

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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm



Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail

sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

# **Body Protection**

Complete suit protecting against chemicals, 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 particle respirator type N100 (US) or type P3 (EN 143) 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

Do not let product enter drains.

# **SECTION 9: Physical and chemical properties**

# 9.1 Information on basic physical and chemical properties

a) Appearance Form: crystalline

Color: yellowyellow

b) Odor stinging

c) Odor Threshold No data availabled) pH No data available

e) Melting point/range: 71 - 74 °C (160 - 165 °F) - lit.

point/freezing point

f) Initial boiling point 202 - 205 °C 396 - 401 °F at 140 hPa - lit. and boiling range

g) Flash point 102 °C (216 °F) - closed cup

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 availablel) Vapor density No data availablem) Density No data available



Relative density No data available n) Water solubility (decomposition)

o) Partition coefficient: log Pow: 1.25 - Bioaccumulation is not expected.

n-octanol/water

p) Autoignition No data available

temperature

q) Decomposition No data available

temperature

r) Viscosity No data availables) Explosive properties No data available

t) Oxidizing properties none

# 9.2 Other safety information

Solubility in other Alcohol at 20 °C (68 °F) - decomposes

solvents Ether at 20 °C (68 °F) - soluble

# **SECTION 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

No data available

#### 10.4 Conditions to avoid

Avoid moisture.

## 10.5 Incompatible materials

Water, Alcohols, Oxidizing agents, Strong bases

#### 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 - 5,600 mg/kg

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

LD50 Oral - Mouse - 3,440 mg/kg Remarks: Behavioral:Muscle weakness.

Behavioral: Ataxia.

Behavioral: Muscle contraction or spasticity.

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

respiratory tract

Inhalation: Corrosive to respiratory system.



Dermal: No data available

# Skin corrosion/irritation

Causes skin burns.

# Serious eye damage/eye irritation

Causes serious eye damage. Causes serious eye damage.

# Respiratory or skin sensitization

No data available

# Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: positive Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Result: Positive results were obtained in some in vitro tests.

Test Type: Mutagenicity (mammal cell test):

Result: negative Remarks: (Lit.)

# 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

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea To the best of our knowledge, the chemical, physical, and toxicological properties have not

been thoroughly investigated.

Decomposition of the substance with tissue moisture.

The following applies to aromatic nitro compounds in general: systemic effect: methaemoglobinaemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

Other dangerous properties can not be excluded.



Handle in accordance with good industrial hygiene and safety practice.

# **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

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

#### 12.6 Other adverse effects

Discharge into the environment must be avoided.

Stability in water

Remarks: Hydrolyzes on contact with water.

# **SECTION 13: Disposal considerations**

#### 13.1 Waste treatment methods

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

# Contaminated packaging

Dispose of as unused product.

## **SECTION 14: Transport information**

# DOT (US)

UN number: 3261 Class: 8 Packing group: II

Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-nitrobenzoyl chloride)

Reportable Quantity (RQ): Poison Inhalation Hazard: No

# **IMDG**

UN number: 3261 Class: 8 Packing group: II EMS-No: F-A, S-B Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-nitrobenzoyl

chloride)

#### **IATA**

UN number: 3261 Class: 8 Packing group: II

Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-nitrobenzoyl chloride)

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# **SECTION 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**

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.

## **Massachusetts Right To Know Components**

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

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

# **Pennsylvania Right To Know Components**

4-nitrobenzoyl chloride CAS-No. Revision Date

122-04-3

# **New Jersey Right To Know Components**

4-nitrobenzoyl chloride CAS-No. Revision Date 122-04-3

#### **SECTION 16: Other information**

#### **Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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