

## SAFETY DATA SHEET

Version 6.2  
Revision Date 10/08/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Phenylbutyryl chloride

Product Number : 349666  
Brand : Aldrich  
CAS-No. : 36854-57-6

**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.

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Precautionary statement(s) |                                                                                                                                  |
| 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                | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.                                 |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P310                       | Immediately call a POISON CENTER/ doctor.                                                                                        |
| P321                       | Specific treatment (see supplemental first aid instructions on this label).                                                      |
| 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 - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                       |
|------------------|---------------------------------------|
| Formula          | : C <sub>10</sub> H <sub>11</sub> ClO |
| Molecular weight | : 182.65 g/mol                        |
| CAS-No.          | : 36854-57-6                          |
| EC-No.           | : 253-241-0                           |

| Component                       | Classification                        | Concentration |
|---------------------------------|---------------------------------------|---------------|
| <b>2-Phenylbutyryl chloride</b> |                                       |               |
|                                 | Skin Corr. 1B; Eye Dam. 1; H314, H318 | <= 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

Consult a physician. Show this material 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

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

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**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

Hydrogen chloride gas

Carbon oxides

Hydrogen chloride gas

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

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

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

**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**

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Avoid inhalation of vapor or mist.

### **Advice on protection against fire and explosion**

Normal measures for preventive fire protection.

### **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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

### **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

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## **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**

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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, 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

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: clear, liquid<br>Color: colorless    |
| b) Odor                                         | No data available                          |
| 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      | 122 - 125 °C 252 - 257 °F at 27 hPa - lit. |
| g) Flash point                                  | 98 °C (208 °F) - closed cup                |
| h) Evaporation rate                             | No data available                          |
| i) Flammability (solid, gas)                    | No data available                          |
| j) Upper/lower flammability or explosive limits | No data available                          |
| k) Vapor pressure                               | No data available                          |
| l) Vapor density                                | No data available                          |
| m) Density                                      | 1.093 g/mL at 25 °C (77 °F) - lit.         |
| Relative density                                | No data available                          |
| n) Water solubility                             | No data available                          |
| o) Partition coefficient: n-octanol/water       | No data available                          |
| 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                         | No data available                          |

#### 9.2 Other safety information

No data available

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### SECTION 10: Stability and reactivity

#### 10.1 Reactivity

No data available

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## **10.2 Chemical stability**

Stable under recommended storage conditions.

## **10.3 Possibility of hazardous reactions**

No data available

## **10.4 Conditions to avoid**

No data available

## **10.5 Incompatible materials**

Strong oxidizing agents

## **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**

Oral: 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 sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **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.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

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., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**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 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**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 3265    Class: 8    Packing group: II  
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (2-Phenylbutyryl chloride)  
Poison Inhalation Hazard: No

### IMDG

UN number: 3265    Class: 8    Packing group: II    EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (2-Phenylbutyryl chloride)

### IATA

UN number: 3265    Class: 8    Packing group: II  
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (2-Phenylbutyryl 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.

### SARA 311/312 Hazards

Acute Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

|                          |                       |               |
|--------------------------|-----------------------|---------------|
| 2-Phenylbutyryl chloride | CAS-No.<br>36854-57-6 | Revision Date |
|--------------------------|-----------------------|---------------|

### New Jersey Right To Know Components

|                          |                       |               |
|--------------------------|-----------------------|---------------|
| 2-Phenylbutyryl chloride | CAS-No.<br>36854-57-6 | Revision Date |
|--------------------------|-----------------------|---------------|

### California Prop. 65 Components

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

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## 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

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