

ALFAAA10860

## 3-Phenylpropionyl chloride

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

<b>产品说明:</b> Product Description:	<b>3-苯基丙酰氯, 98%</b> 3-Phenylpropionyl chloride
<b>Cat No. :</b>	<b>A10860</b>
<b>Synonyms</b>	3-Phenylpropionyl chloride
<b>CAS No</b>	645-45-4
<b>Molecular Formula</b>	C9 H9 Cl O
<b>Supplier</b>	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
<b>Emergency Telephone Number</b>	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US</b> :001-201-796-7100 / <b>Europe</b> : +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US</b> :001-800-424-9300 / <b>Europe</b> :001-703-527-3887
<b>E-mail address</b>	begel.sdsdesk@thermofisher.com
<b>Recommended Use</b>	Laboratory chemicals.
<b>Uses advised against</b>	No Information available

### SECTION 2. HAZARD IDENTIFICATION

<b>Physical State</b> Liquid	<b>Appearance</b> Light yellow	<b>Odor</b> pungent
<b>Emergency Overview</b> Causes skin irritation. Toxic if inhaled. Harmful to aquatic life with long lasting effects. Moisture sensitive.		

#### Classification of the substance or mixture

Acute Inhalation Toxicity - Vapors	Category 3
Skin Corrosion/Irritation	Category 2
Chronic aquatic toxicity	Category 3

#### Label Elements



**Signal Word**

**Danger**

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**Hazard Statements**

H315 - Causes skin irritation  
H331 - Toxic if inhaled  
H412 - Harmful to aquatic life with long lasting effects

**Precautionary Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P273 - Avoid release to the environment

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep 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  
P311 - Call a POISON CENTER or doctor  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**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

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Causes skin irritation. Toxic if inhaled.

**Environmental hazards**

Harmful to aquatic life with long lasting effects. Is not likely mobile in the environment. Decomposes in contact with water.

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
Benzenepropanoyl chloride	645-45-4	<=100

**SECTION 4. FIRST AID MEASURES****General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms and effects**

None reasonably foreseeable. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible

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perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam.

**Extinguishing media which must not be used for safety reasons**

Contact with water liberates toxic gas.

**Specific Hazards Arising from the Chemical**

Contact with water liberates toxic gas.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

**Environmental Precautions**

Should not be released into the environment. Do not flush into surface water or sanitary sewer system.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Do not expose spill to water.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water.

**Storage**

Keep away from water or moist air. Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters**

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**Exposure Controls****Engineering Measures**

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** Prevent product from entering drains.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

<b>Appearance</b>	Light yellow
<b>Physical State</b>	Liquid
<b>Odor</b>	pungent
<b>Odor Threshold</b>	No data available
<b>pH</b>	Not applicable
<b>Melting Point/Range</b>	-6 - -5.00 °C / 21.2 - 23 °F
<b>Softening Point</b>	No data available
<b>Boiling Point/Range</b>	107 °C / 224.6 °F @ 11 mmHg

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<b>Flash Point</b>	108 °C / 226.4 °F	<b>Method</b> - No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	5.81	(Air = 1.0)
<b>Specific Gravity / Density</b>	1.137	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	Decomposes in contact with water	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	No data available	
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C9 H9 Cl O	
<b>Molecular Weight</b>	168.62	

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Moisture sensitive.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Conditions to Avoid</b>	Incompatible products. Excess heat. Exposure to moist air or water. Exposure to moisture.
<b>Materials to avoid</b>	Strong oxidizing agents.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen chloride gas.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenepropanoyl chloride			2750 mg/m <sup>3</sup> /4h (Rat)

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; No data available

## (d) respiratory or skin sensitization;

Respiratory No data available  
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

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(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs None known.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

## SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains. Reacts with water so no ecotoxicity data for the substance is available. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Benzenepropanoyl chloride			Desmodesmus subspicatus: EC50 = 56 mg/L (72 h)	

Persistence and Degradability No information available  
Persistence Persistence is unlikely, based on information available.  
Degradability Decomposes in contact with water.  
Degradation in sewage treatment plant No information available. Decomposes in contact with water. Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential Product does not bioaccumulate due to reaction with water

Mobility in soil Decomposes in contact with water Is not likely mobile in the environment

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors  
Persistent Organic Pollutant This product does not contain any known or suspected substance  
Ozone Depletion Potential This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms. Do not let this chemical enter the environment.

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## SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

**UN-No** UN2810  
**Proper Shipping Name** TOXIC LIQUID, ORGANIC, N.O.S.  
**Technical Shipping Name** Hydrocinnamoyl chloride  
**Hazard Class** 6.1  
**Packing Group** III

IMDG/IMO

**UN-No** UN2810  
**Proper Shipping Name** TOXIC LIQUID, ORGANIC, N.O.S.  
**Technical Shipping Name** Hydrocinnamoyl chloride  
**Hazard Class** 6.1  
**Packing Group** III

IATA

**UN-No** UN2810  
**Proper Shipping Name** TOXIC LIQUID, ORGANIC, N.O.S.  
**Technical Shipping Name** Hydrocinnamoyl chloride  
**Hazard Class** 6.1  
**Packing Group** III

**Special Precautions for User** No special precautions required

## SECTION 15. REGULATORY INFORMATION

**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Benzenepropanoyl chloride	-	-	X	-	211-443-6	X	-	X	-	X	X	-

**National Regulations**

## SECTION 16. OTHER INFORMATION

**Prepared By** Health, Safety and Environmental Department  
**Creation Date** 20-Sep-2010  
**Revision Date** 22-Apr-2024  
**Revision Summary** New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

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Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**