

ALFAAA10860

3-Phenylpropionyl chloride

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

产品说明:
Product Description: 3-苯基丙酰氯, 98%
3-Phenylpropionyl chloride

Cat No. : A10860
Synonyms 3-Phenylpropionyl chloride
CAS No 645-45-4
Molecular Formula C9 H9 Cl O

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Light yellow

Odor
pungent

Emergency Overview

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**

CO₂, 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	-	EN 374	(minimum requirement)
Neoprene	recommendations			
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 compatability, 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

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

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

SECTION 10. STABILITY AND REACTIVITY

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

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen chloride gas.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenepropanoyl chloride			2750 mg/m ³ /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