

SAFETY DATA SHEET

Creation Date 20-Sep-2010

Revision Date 25-Mar-2024

Revision Number 4

1. Identification

Product Name 3-Phenylpropionyl chloride
Cat No. : A10860
CAS No 645-45-4
Synonyms 3-Phenylpropionyl chloride
Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
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

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute Inhalation Toxicity - Vapors	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2

Label Elements

Signal Word

Danger

Hazard Statements

Causes skin irritation
Causes serious eye irritation
Toxic if inhaled

**Precautionary Statements****Prevention**

Avoid breathing dust/fume/gas/mist/vapors/spray

Use only outdoors or in a well-ventilated area

Wash face, hands and any exposed skin thoroughly after handling

Wear protective gloves/protective clothing/eye protection/face protection

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Call a POISON CENTER or doctor/physician

Skin

IF ON SKIN: Wash with plenty of soap and water

If skin irritation occurs: Get medical advice/attention

Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

If eye irritation persists: Get medical advice/attention

Storage

Store in a well-ventilated place. Keep container tightly closed

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Harmful to aquatic life with long lasting effects

3. Composition/Information on Ingredients

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

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 perforation of stomach or esophagus should be

Notes to Physician investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media CO₂, dry chemical, dry sand, alcohol-resistant foam.

Unsuitable Extinguishing Media DO NOT USE WATER

Flash Point 108 °C / 226.4 °F

Method - No information available

Autoignition Temperature No information available

Explosion Limits

Upper No data available

Lower No data available

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Contact with water liberates toxic gas.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen chloride 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.

NFPA

Health
3

Flammability
1

Instability
2

Physical hazards
W

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.

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. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

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

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 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.

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

9. Physical and chemical properties

Physical State	Liquid
Appearance	Light yellow
Odor	pungent
Odor Threshold	No information available
pH	Not applicable
Melting Point/Range	-6 - -5.00 °C / 21.2 - 23 °F
Boiling Point/Range	107 °C / 224.6 °F @ 11 mmHg
Flash Point	108 °C / 226.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	5.81
Specific Gravity	1.137
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C9 H9 Cl O
Molecular Weight	168.62

10. Stability and reactivity

Reactive Hazard Yes

Stability Moisture sensitive.

Conditions to Avoid Incompatible products. Excess heat. Exposure to moist air or water. Exposure to moisture.

Incompatible Materials Strong oxidizing agents

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

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenepropanoyl chloride	Not listed	Not listed	2750 mg/m ³ /4h (Rat)

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Benzenepropanoyl chloride	645-45-4	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard No information available

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

Endocrine Disruptor Information No information available

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

12. Ecological information

Ecotoxicity

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 Algae	Freshwater Fish	Microtox	Water Flea
Benzenepropanoyl chloride	Desmodesmus subspicatus: EC50 = 56 mg/L (72 h)	Not listed	Not listed	Not listed

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Is not likely mobile in the environment.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

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

TDG

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

IATA

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

IMDG/IMO

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

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzenepropanoyl chloride	645-45-4	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzenepropanoyl chloride	645-45-4	-	X	211-443-6	X	-	X	X	-	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any

chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Benzenepropanoyl chloride	645-45-4	-	-	-

Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Benzenepropanoyl chloride	645-45-4	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Benzenepropanoyl chloride	645-45-4	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By	Health, Safety and Environmental Department Email: chem.techinfo@thermofisher.com www.thermofisher.com
Creation Date	20-Sep-2010
Revision Date	25-Mar-2024
Print Date	25-Mar-2024
Revision Summary	New emergency telephone response service provider.

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 SDS