

SAFETY DATA SHEET

Creation Date 22-May-2015

Revision Date 20-Dec-2025

Revision Number 3

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name	3-Phenylpropyl isocyanate, 97%
Cat No. :	AC457380000; AC457380010; AC457380050
CAS No	68664-23-3
Synonyms	No information available
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

CHEMTRAC®, Inside the USA: 800-424-9300
CHEMTRAC®, Outside the USA: 001-703-527-3887
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
CHEMTRAC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements**Signal Word**

Danger

Hazard Statements

Causes skin irritation
Causes serious eye irritation
May cause an allergic skin reaction
May cause allergy or asthma symptoms or breathing difficulties if inhaled
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
In case of inadequate ventilation wear respiratory protection
Contaminated work clothing should not be allowed out of the workplace

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
If experiencing respiratory symptoms: Call a POISON CENTER or doctor

Skin

IF ON SKIN: Wash with plenty of soap and water
Call a POISON CENTER or doctor if you feel unwell
Take off contaminated clothing

If skin irritation or rash occurs: Get medical advice/attention

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

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

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)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
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3-Phenylpropyl isocyanate	68664-23-3	<=100
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4. First-aid measures

General Advice	If symptoms persist, call a physician.
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. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
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

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

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.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	0	N/A

6. Accidental release measures

Personal Precautions	Use personal protective equipment as required. Ensure adequate ventilation.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

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7. Handling and Storage

Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.
Storage.	Keep containers tightly closed in a dry, cool and well-ventilated place. To maintain product quality. Air sensitive. Store under an inert atmosphere. Incompatible Materials. Water. Strong oxidizing agents. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limitsestablished by the region specific regulatory bodies.
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Engineering Measures	Ensure that eyewash stations and safety showers are close to the workstation location.
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Personal Protective Equipment

Eye/face Protection	Tight sealing safety goggles. Face protection shield.
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

Appearance

Physical State	Liquid		
Color	Clear Pale yellow		
Odor	No information available		
Odor Threshold	No information available		
Property	Values	Remarks	• Method
Melting Point/Range	238 - 239 °C / 460.4 - 462.2 °F		
Softening Point	No data available		
Boiling Point/Range	245 °C / 473 °F	@ 12 mmHg	
Flash Point	No information available	Method - No information available	
Flammability (liquid)	No data available		
Flammability (solid,gas)	Not applicable		
Explosion Limits	No data available	Liquid	
Autoignition Temperature	No data available		
Decomposition Temperature	No data available		
pH	No information available		
Viscosity	No data available		
Water Solubility	No information available		
Solubility in other solvents	No information available		
Partition Coefficient (n-octanol/water)			
Vapor Pressure	No data available		
Density / Specific Gravity	No data available		

Bulk Density	Not applicable	Liquid (Air = 1.0)
Vapor Density	No data available	
Particle characteristics	Not applicable (liquid)	

Other Information

Molecular Formula	C10H11NO
Molecular Weight	161.21

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under recommended storage conditions. Moisture sensitive.
Conditions to Avoid	Incompatible products. Excess heat.
Incompatible Materials	Water, Strong oxidizing agents, Strong bases
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Nitrogen oxides (NO _x)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information**Information on expected route of exposure**

Inhalation	May cause irritation of respiratory tract.
Ingestion	Ingestion may cause irritation to mucous membranes.
Eyes	Irritating to eyes. Contact with eyes may cause irritation.
Skin	Irritating to skin. Repeated or prolonged skin contact may cause allergic reactions with susceptible persons. May cause eye/skin irritation.

Toxicology data for the components

Toxicologically Synergistic Products	No information available
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(b) skin corrosion/irritation;	Category 2
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(c) serious eye damage/irritation;	Category 2
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(d) respiratory or skin sensitization;	
Respiratory	Category 1
Skin	Category 1

No information available

(e) germ cell mutagenicity;	No data available
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(f) carcinogenicity;

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
3-Phenylpropyl	68664-23-3	Not listed				

isocyanate					
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(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects,both acute and delayed Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

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

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

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability No information available

Bioaccumulation/ Accumulation No information available.

Mobility No information available.

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 UN2206
Proper Shipping Name Isocyanates, toxic, n.o.s.
Technical Shipping Name 3-Phenylpropyl isocyanate
Hazard Class 6.1
Packing Group III

TDG

UN-No UN2206
Proper Shipping Name Isocyanate solution, toxic, n.o.s.
Technical Shipping Name 3-Phenylpropyl isocyanate
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2206
Proper Shipping Name Isocyanate solution, toxic, n.o.s.
Technical Shipping Name 3-Phenylpropyl isocyanate
Hazard Class 6.1

Packing Group	III
IMDG/IMO	
UN-No	UN2206
Proper Shipping Name	Isocyanates, toxic, n.o.s.
Technical Shipping Name	3-Phenylpropyl isocyanate
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
3-Phenylpropyl isocyanate	68664-23-3	-	-	-

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
3-Phenylpropyl isocyanate	68664-23-3	-	-	-	-	-	-	-	-	-

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)
3-Phenylpropyl isocyanate	68664-23-3	-	-	-

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)
3-Phenylpropyl isocyanate	68664-23-3	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)
3-Phenylpropyl isocyanate	68664-23-3	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By Product stewardship (Regulatory Affairs)
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Revision Summary Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard

Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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