

SAFETY DATA SHEET

Creation Date 22-May-2015

Revision Date 24-Dec-2021

Revision Number 2

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 CHEMTREC®, Inside the USA: 800-424-9300
CHEMTREC®, Outside the USA: 001-703-527-3887
For information **US** call: 001-800-ACROS-01 / **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 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 victim to fresh air and keep at rest in a position comfortable for breathing

If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician

Skin

IF ON SKIN: Wash with plenty of soap and water

Call a POISON CENTER or doctor/physician if you feel unwell

Take off contaminated clothing and wash before reuse

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

3. Composition/Information on Ingredients

Component	CAS No	Weight %
3-Phenylpropyl isocyanate	68664-23-3	<=100

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
2

Flammability
1

Instability
0

Physical hazards
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 Up Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

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. Protect from moisture. 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 limits established by the region specific regulatory bodies.
Engineering Measures	Ensure that eyewash stations and safety showers are close to the workstation location.
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.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear Pale yellow
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	238 - 239 °C / 460.4 - 462.2 °F
Boiling Point/Range	245 °C / 473 °F @ 12 mmHg
Flash Point	No information available
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	No information available
Specific Gravity	No information available
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	C ₁₀ H ₁₁ NO
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

Acute Toxicity

Product Information

Component Information

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
3-Phenylpropyl isocyanate	68664-23-3	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	Respiratory system
STOT - repeated exposure	None known
Aspiration hazard	No information 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
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.

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 Name 3-Phenylpropyl isocyanate
 Hazard Class 6.1
 Packing Group III

TDG

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

IATA

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

IMDG/IMO

UN-No UN2206
 Proper Shipping Name Isocyanates, toxic, 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
3-Phenylpropyl isocyanate	68664-23-3	-	-	-

Legend:

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

X - Listed

'-' - Not Listed

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 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

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

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

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 Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date 22-May-2015

Revision Date 24-Dec-2021

Print Date 24-Dec-2021

Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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