

# SAFETY DATA SHEET

Revision Date 19-Dec-2025

Revision Number 5

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** Pentyl isocyanate

**Cat No. :** AC314320000; AC314320010; AC314320050

**CAS No** 3954-13-0  
**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**

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 according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 3
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 1
Respiratory Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

### Label Elements

**Signal Word**

Danger

**Hazard Statements**

Flammable liquid and vapor  
Causes skin irritation  
Causes serious eye damage  
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  
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
Keep container tightly closed  
Ground and bond container and receiving equipment  
Use explosion-proof electrical/ventilating/lighting equipment  
Keep cool  
Take action to prevent static discharges  
Use non-sparking tools

**Inhalation**

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

**Skin**

Call a POISON CENTER or doctor if you feel unwell  
If skin irritation occurs: Get medical advice/attention  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
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  
Immediately call a POISON CENTER or doctor/physician

**Ingestion**

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

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam to extinguish

**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 %
Pentyl isocyanate	3954-13-0	<=100

### 4. First-aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
<b>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
<b>Ingestion</b>	Clean mouth with water. Get medical attention.
<b>Most important symptoms and effects</b>	Difficulty in breathing. Causes eye burns. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Causes severe eye damage. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting; 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
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	32 °C / 89.6 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

#### Specific Hazards Arising from the Chemical

Flammable. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

#### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid).

#### 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**  
2

**Instability**  
0

**Physical hazards**  
N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	See Section 12 for additional Ecological Information.
<b>Methods for Containment and Clean Up</b>	Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not let this chemical enter the environment.

## 7. Handling and Storage

<b>Handling</b>	Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges.
<b>Storage.</b>	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place. Incompatible Materials. Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines.

## 8. Exposure controls / personal protection

<b>Exposure Guidelines</b>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
<b>Engineering Measures</b>	Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.
<b>Personal Protective Equipment</b>	
<b>Eye/face Protection</b>	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.
<b>Skin and body protection</b>	Wear appropriate protective gloves and clothing to prevent skin exposure.
<b>Respiratory Protection</b>	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.
<b>Recommended Filter type:</b>	Organic gases and vapours filter. Type A. Brown. conforming to EN14387.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

<b>Appearance</b>			
<b>Physical State</b>	Liquid		
<b>Color</b>	Colorless		
<b>Odor</b>	No information available		
<b>Odor Threshold</b>	No information available		
<b>Property</b>	<b>Values</b>	<b>Remarks</b>	<b>Method</b>
<b>Melting Point/Range</b>	No data available		
<b>Softening Point</b>	No data available		
<b>Boiling Point/Range</b>	136 - 137 °C / 276.8 - 278.6 °F	@ 760 mmHg	

<b>Flash Point</b>	32 °C / 89.6 °F	<b>Method</b> - No information available
<b>Flammability (liquid)</b>	Flammable	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	0.870	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	
<b>Other Information</b>		
<b>Molecular Formula</b>	C6 H11 N O	
<b>Molecular Weight</b>	113.16	
<b>Explosive Properties</b>	explosive air/vapour mixtures possible	

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Moisture sensitive.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition. Excess heat. Incompatible products. Exposure to moist air or water.
<b>Incompatible Materials</b>	Acids, Strong oxidizing agents, Strong bases, Alcohols, Amines
<b>Hazardous Decomposition Products</b>	Nitrogen oxides (NO <sub>x</sub> ), Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Hydrogen cyanide (hydrocyanic acid)
<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Information on expected route of exposure

<b>Inhalation</b>	Not an expected route of exposure.
<b>Ingestion</b>	May be harmful if swallowed.
<b>Eyes</b>	Avoid contact with eyes. Corrosive to the eyes and may cause severe damage including blindness. May cause irritation. Lachrymator (substance which increases the flow of tears).
<b>Skin</b>	Avoid contact with skin. Skin Corrosion/Irritation. May cause irritation. Harmful in contact with skin.

### Toxicology data for the components

<b>Toxicologically Synergistic Products</b>	No information available
<b>(b) skin corrosion/irritation;</b>	Category 2

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory Category 1  
 Skin No data available  
 No information available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Pentyl isocyanate	3954-13-0	Not listed				

(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

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

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. 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**

<b>UN-No</b>	UN3080
<b>Proper Shipping Name</b>	Isocyanates, toxic, flammable, n.o.s.
<b>Technical Shipping Name</b>	Pentyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	3
<b>Packing Group</b>	II

**TDG**

<b>UN-No</b>	UN3080
<b>Proper Shipping Name</b>	Isocyanate solution, toxic, flammable, n.o.s.
<b>Technical Shipping Name</b>	Pentyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	3
<b>Packing Group</b>	II

**IATA**

<b>UN-No</b>	UN3080
<b>Proper Shipping Name</b>	Isocyanate solution, toxic, flammable, n.o.s.
<b>Technical Shipping Name</b>	Pentyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	3
<b>Packing Group</b>	II

**IMDG/IMO**

<b>UN-No</b>	UN3080
<b>Proper Shipping Name</b>	Isocyanates, toxic, flammable, n.o.s.
<b>Technical Shipping Name</b>	Pentyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	3
<b>Packing Group</b>	II

## 15. Regulatory Information

**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Pentyl isocyanate	3954-13-0	-	-	-

**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
Pentyl isocyanate	3954-13-0	-	-	-	-	-	-	-	-	-

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)
Pentyl isocyanate	3954-13-0	-	-	-

**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)
Pentyl isocyanate	3954-13-0	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)
Pentyl isocyanate	3954-13-0	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other Information

<b>Prepared By</b>	Product stewardship (Regulatory Affairs) Thermo Fisher Scientific email - begel.sdsdesk@thermofisher.com
<b>Revision Date</b>	19-Dec-2025
<b>Print Date</b>	19-Dec-2025
<b>Revision Summary</b>	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**