

## SAFETY DATA SHEET

Revision Date 30-Mar-2024

Revision Number 3

### 1. Identification

**Product Name** 3-(1-Cyanoethyl)benzoic acid  
**Cat No. :** H60537  
**CAS No** 5537-71-3  
**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

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)

Serious Eye Damage/Eye Irritation

Category 2

#### Label Elements

##### **Signal Word**

Warning

##### **Hazard Statements**

Causes serious eye irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Wear eye/face protection

**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

**Hazards not otherwise classified (HNOC)**

None identified

### 3. Composition/Information on Ingredients

Component	CAS No	Weight %
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	<=100

### 4. First-aid measures

<b>General Advice</b>	If symptoms persist, call a physician.
<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 plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
<b>Most important symptoms and effects</b>	None reasonably foreseeable.
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Carbon dioxide (CO <sub>2</sub> ). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	No information available
<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**

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

**Hazardous Combustion Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</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**  
0

**Instability**  
0

**Physical hazards**  
-

**6. Accidental release measures**

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.
<b>Environmental Precautions</b>	Should not be released into the environment. See Section 12 for additional Ecological Information.
<b>Methods for Containment and Clean Up</b>	Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

**7. Handling and storage**

<b>Handling</b>	Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Avoid dust formation. Do not get in eyes, on skin, or on clothing.
<b>Storage.</b>	Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong bases. Oxidizing agent.

**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>	None under normal use conditions. Ensure that eyewash stations and safety showers are close to the workstation location.
<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>	No protective equipment is needed under normal use conditions.
<b>Recommended Filter type:</b>	Particle filter.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

**9. Physical and chemical properties**

Physical State	Solid
Appearance	No information available
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	145 - 148 °C / 293 - 298.4 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
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	Not applicable
Molecular Formula	C10 H9 N O2
Molecular Weight	175.18

## 10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Strong bases, Oxidizing agent
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Nitrogen oxides (NO <sub>x</sub> ), Hydrogen cyanide (hydrocyanic acid)
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
Benzoic acid, 3-(1-cyanoethyl)-	Not listed	LD50 > 2000 mg/kg ( Rat )	Not listed

**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
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Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	Not listed	Not listed	Not listed	Not listed	Not listed
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**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** No information available

**Endocrine Disruptor Information** No information available

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

## 12. Ecological information

### Ecotoxicity

**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** Not regulated

**TDG** Not regulated

**IATA** Not regulated

**IMDG/IMO** Not regulated

## 15. Regulatory information

### United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	-	-	-

#### **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
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	X	-	226-897-0	-	-		-	-	KE-05-0376

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	REACH Regulation (EC 1907/2006) article 59 - Candidate List of

			Substances	Substances of Very High Concern (SVHC)
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	-	-	-

**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)
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	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)
Benzoic acid, 3-(1-cyanoethyl)-	5537-71-3	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other information

**Prepared By**

Health, Safety and Environmental Department  
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 www.thermofisher.com

**Revision Date**

30-Mar-2024

**Print Date**

30-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**