

SAFETY DATA SHEET

Revision Date 22-Dec-2025

Revision Number 4

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-Acetylbenzotrile
Cat No. : A10841
CAS No 6136-68-1
Synonyms 3'-Cyanoacetophenone
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 according to [US] OSHA (29 CFR 1910.1200, 2024)

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Dusts and Mists	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	
Combustible dust	Yes

Label Elements

Signal Word

Warning

Hazard Statements

May form combustible dust concentrations in air
 Causes skin irritation
 Causes serious eye irritation
 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

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
 Call a POISON CENTER or doctor if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
 Call a POISON CENTER or doctor if you feel unwell
 If skin irritation occurs: Get medical advice/attention
 Take off contaminated clothing

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 %
3-Acetylbenzotrile	6136-68-1	<=100

4. First-aid measures

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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
Ingestion	Clean mouth with water. Get medical attention.
Most important symptoms and effects	No information available.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Chemical 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

Fine dust dispersed in air may ignite.

Hazardous Combustion Products

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

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	Ensure adequate ventilation. Use personal protective equipment as required.
Environmental Precautions	See Section 12 for additional Ecological Information.
Methods for Containment and Clean Up	Avoid dust formation. Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

7. Handling and Storage

Handling	Avoid contact with skin and eyes. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.
Storage.	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible Materials. Acids. Strong oxidizing agents. Strong bases. Reducing Agent.

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 adequate ventilation, especially in confined areas. 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:	Particulates filter conforming to EN 143.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance			
Physical State	Powder Solid		
Color	Amber		
Odor	No information available		
Odor Threshold	No information available		
Property	Values	Remarks	Method
Melting Point/Range	96 - 100 °C / 204.8 - 212 °F		
Softening Point	No data available		
Boiling Point/Range	120 °C / 248 °F	@ 5 mmHg	
Flash Point	No information available	Method -	No information available
Flammability (liquid)	Not applicable	Solid	
Flammability (solid,gas)	No information available		
Explosion Limits	No data available		
Autoignition Temperature	No data available		
Decomposition Temperature	No data available		
pH	No information available		
Viscosity	Not applicable	Solid	
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	No data available		
Vapor Density	Not applicable	Solid	
Particle characteristics	No data available		
Other Information			
Molecular Formula	C9 H7 N O		
Molecular Weight	145.16		
Evaporation Rate	Not applicable - Solid		

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Acids, Strong oxidizing agents, Strong bases, Reducing Agent
Hazardous Decomposition Products	Nitrogen oxides (NO _x), Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Harmful by inhalation. Avoid breathing dust or spray mist.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes. Irritating to eyes.
Skin	Avoid contact with skin. May cause irritation. Harmful in contact with skin.

Toxicology data for the components

Toxicologically Synergistic Products No information available

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data 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
3-Acetylbenzotrile	6136-68-1	Not listed	Not listed	Not listed	Not listed	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;	Not applicable Solid
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	No information available.
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	UN3439
Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class	6.1
Packing Group	III

TDG

UN-No	UN3439
Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class	6.1
Packing Group	III

IATA

UN-No	UN3439
Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class	6.1
Packing Group	III

IMDG/IMO

UN-No	UN3439
Proper Shipping Name	NITRILES, SOLID, 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-Acetylbenzotrile	6136-68-1	-	-	-

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-Acetylbenzotrile	6136-68-1	-	-	228-110-6	-	-		-	-	-

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 This product does not contain any DHS chemicals.

Security**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-Acetylbenzotrile	6136-68-1	-	-	-

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-Acetylbenzotrile	6136-68-1	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-Acetylbenzotrile	6136-68-1	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

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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