

SAFETY DATA SHEET

Creation Date 14-May-2010

Revision Date 19-Dec-2025

Revision Number 6

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 | p-Tolunitrile |
| Cat No. : | AC158020000; AC158020010; AC158020050; AC158021000; AC158022500 |
| CAS No | 104-85-8 |
| Synonyms | 4-Methylbenzenecarbonitrile; CNT |
| 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 | Acros Organics |
| One Reagent Lane | One Reagent Lane |
| Fair Lawn, NJ 07410 | Fair Lawn, NJ 07410 |
| Tel: (201) 796-7100 | |

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 4 |
| Skin Corrosion/Irritation | Category 2 |
| Serious Eye Damage/Eye Irritation | Category 2 |
| Respiratory Sensitization | Category 1 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Respiratory system. | |

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid
Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
In case of inadequate ventilation wear respiratory protection
Use only outdoors or in a well-ventilated area
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

Keep cool

Inhalation

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

Skin

IF ON SKIN: Wash with plenty of soap and water
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

Fire

In case of fire: Use CO₂, 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 % |
|-------------------------|----------|----------|
| Benzonitrile, 4-methyl- | 104-85-8 | <=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 | Irritating to respiratory system. |
| Notes to Physician | Treat symptomatically |

5. Fire-fighting measures

| | |
|-----------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Suitable Extinguishing Media | Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers. |
| Unsuitable Extinguishing Media | No information available |
| Flash Point | 85 °C / 185 °F |
| 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

Combustible material. Containers may explode when heated.

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
2

Flammability
2

Instability
0

Physical hazards
N/A

6. Accidental release measures

| | |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Personal Precautions | Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges. |
| Environmental Precautions | Should not be released into the environment. |

| | |
|---------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| Methods for Containment and Clean Up | Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. |
|---------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|

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. Keep away from open flames, hot surfaces and sources of ignition. |
| Storage. | Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from |

heat, sparks and flame. Incompatible Materials. Strong oxidizing agents. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

| Component | ACGIH TLV | OSHA PEL | NIOSH | Mexico OEL (TWA) |
|-------------------------|-----------|------------------------------------|----------------------------|------------------|
| Benzonitrile, 4-methyl- | | (Vacated) TWA: 5 mg/m ³ | IDLH: 25 mg/m ³ | |

Legend

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

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

Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions.

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

Odor

Odorless

Odor Threshold

No information available

Property

Values

Remarks

• Method

Melting Point/Range

26 - 28 °C / 78.8 - 82.4 °F

Softening Point

No data available

Boiling Point/Range

103 - 106 °C / 217.4 - 222.8 °F

@ 20 mmHg

Flash Point

85 °C / 185 °F

Method - No information available

Flammability (liquid)

Combustible liquid

On basis of test data

Flammability (solid,gas)

Not applicable

Liquid

Explosion Limits

No data available

Autoignition Temperature

No data available

Decomposition Temperature

No data available

pH

No information available

Viscosity

No data available

Water Solubility

Insoluble

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

Vapor Pressure

0.980

Density / Specific Gravity

Not applicable

Liquid

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

Other Information

Molecular Formula C8 H7 N
Molecular Weight 117.15
Explosive Properties explosive air/vapour mixtures possible

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials Strong oxidizing agents, Strong bases

Hazardous Decomposition Products Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂)

Hazardous Polymerization No information available.

Hazardous Reactions None under normal processing.

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

Inhalation Not an expected route of exposure.

Ingestion May be harmful if swallowed.

Eyes Avoid contact with eyes. Irritating to eyes.

Skin Avoid contact with skin. May cause irritation.

Toxicology data for the components

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|-------------------------|---------------------------|-------------|-----------------|
| Benzonitrile, 4-methyl- | LD50 = 3800 mg/kg (Rat) | - | - |

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 |
|-----------|--------|------|-----|-------|------|--------|
| | | | | | | |

| | | | | | | |
|-------------------------|----------|------------|------------|------------|------------|------------|
| Benzonitrile, 4-methyl- | 104-85-8 | 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

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

Persistence and Degradability Insoluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

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 COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk

UN-No NA1993
Proper Shipping Name Combustible liquid, n.o.s.

Packing Group III

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 |
|-------------------------|----------|------|-----------------------------------------------|-----------------------------|
| Benzonitrile, 4-methyl- | 104-85-8 | X | ACTIVE | - |

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 |
|-------------------------|----------|-----|------|-----------|-------|------|------|------|-------|-------------|
| Benzonitrile, 4-methyl- | 104-85-8 | - | X | 203-244-8 | X | X | X | - | X | 2014-3-5918 |

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 contains a chemical or chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

| Component | CAS No | Weight % | SARA 313 - Threshold Values % | SARA 313 - Reporting thresholds |
|-------------------------|----------|----------|-------------------------------|---------------------------------|
| Benzonitrile, 4-methyl- | 104-85-8 | <=100 | 1.0 % | - |

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)

| Component | CWA - Hazardous Substances | CWA - Reportable Quantities | CWA - Toxic Pollutants | CWA - Priority Pollutants |
|-------------------------|----------------------------|-----------------------------|------------------------|---------------------------|
| Benzonitrile, 4-methyl- | - | - | X | X |

Clean Air Act

| Component | HAPS Data | Class 1 Ozone Depletors | Class 2 Ozone Depletors |
|-------------------------|-----------|-------------------------|-------------------------|
| Benzonitrile, 4-methyl- | X | | - |

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

| Component | Massachusetts | New Jersey | Pennsylvania | Illinois | Rhode Island |
|-----------|---------------|------------|--------------|----------|--------------|
| | | | | | |

| | | | | | |
|-------------------------|---|---|---|---|---|
| Benzonitrile, 4-methyl- | - | X | X | X | X |
|-------------------------|---|---|---|---|---|

U.S. Department of Transportation

Reportable Quantity (RQ): N
 DOT Marine Pollutant Y
 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) |
|-------------------------|----------|---------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Benzonitrile, 4-methyl- | 104-85-8 | - | - | - |

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) |
|-------------------------|----------|----------------|------------------------------|---------------------------|--------------------------------------------|
| Benzonitrile, 4-methyl- | 104-85-8 | 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) |
|-------------------------|----------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|----------------------------|------------------------------------|
| Benzonitrile, 4-methyl- | 104-85-8 | Not applicable | Not applicable | Not applicable | Not applicable |

16. Other Information

Prepared By Product stewardship (Regulatory Affairs)
 Thermo Fisher Scientific
 email - begel.sdsdesk@thermofisher.com

Creation Date 14-May-2010
Revision Date 19-Dec-2025
Print Date 19-Dec-2025
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