

## 1 Identification

### Product identifier

**Product name:** p-Toluenesulfonylacetonitrile

**Stock number:** L04963

**CAS Number:**

5697-44-9

**EC number:**

227-173-7

**Relevant identified uses of the substance or mixture and uses advised against.**

**Identified use:** SU24 Scientific research and development

### Details of the supplier of the safety data sheet

#### Manufacturer/Supplier:

Alfa Aesar

Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

**Information Department:** Health, Safety and Environmental Department

#### Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

## 2 Hazard(s) identification

### Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

**Hazards not otherwise classified** No information known.

### Label elements

**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

### Hazard pictograms



GHS06

### Signal word

Danger

### Hazard statements

H302+H312 Harmful if swallowed or in contact with skin.

H331 Toxic if inhaled.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

### Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

### WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

D2B - Toxic material causing other toxic effects



### Classification system

#### HMIS ratings (scale 0-4)

#### (Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

### Other hazards

### Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

## 3 Composition/information on ingredients

### Chemical characterization: Substances

#### CAS# Description:

5697-44-9 p-Toluenesulfonylacetonitrile

**Product name:** *p*-Toluenesulfonylacetonitrile

**Identification number(s):**  
**EC number:** 227-173-7

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#### 4 First-aid measures

**Description of first aid measures**

**After inhalation**

Supply fresh air. If required, provide artificial respiration. Keep patient warm.  
Seek immediate medical advice.

**After skin contact**

Immediately wash with water and soap and rinse thoroughly.  
Seek immediate medical advice.

**After eye contact** Rinse opened eye for several minutes under running water. Then consult a doctor.

**After swallowing** Seek medical treatment.

**Information for doctor**

**Most important symptoms and effects, both acute and delayed** No further relevant information available.

**Indication of any immediate medical attention and special treatment needed** No further relevant information available.

#### 5 Fire-fighting measures

**Extinguishing media**

**Suitable extinguishing agents** Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

**Special hazards arising from the substance or mixture**

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NO<sub>x</sub>)

Sulfur oxides (SO<sub>x</sub>)

Hydrogen cyanide (HCN)

**Advice for firefighters**

**Protective equipment:**

Wear self-contained respirator.

Wear fully protective impervious suit.

#### 6 Accidental release measures

**Personal precautions, protective equipment and emergency procedures**

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

**Environmental precautions:** Do not allow material to be released to the environment without proper governmental permits.

**Methods and material for containment and cleaning up:**

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

**Prevention of secondary hazards:** No special measures required.

**Reference to other sections**

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

#### 7 Handling and storage

**Handling**

**Precautions for safe handling**

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

**Information about protection against explosions and fires:** No information known.

**Conditions for safe storage, including any incompatibilities**

**Storage**

**Requirements to be met by storerooms and receptacles:** No special requirements.

**Information about storage in one common storage facility:** Store away from oxidizing agents.

**Further information about storage conditions:**

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

**Specific end use(s)** No further relevant information available.

#### 8 Exposure controls/personal protection

**Additional information about design of technical systems:**

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

**Control parameters**

**Components with limit values that require monitoring at the workplace:** Not required.

**Additional information:** No data

**Exposure controls**

**Personal protective equipment**

**General protective and hygienic measures**

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

**Breathing equipment:** Use suitable respirator when high concentrations are present.

**Protection of hands:**

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

**Eye protection:** Safety glasses

**Body protection:** Protective work clothing.

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**9 Physical and chemical properties**

<b>Information on basic physical and chemical properties</b>	
<b>General Information</b>	
<b>Appearance:</b>	
<b>Form:</b>	Crystalline
<b>Odor:</b>	Not determined
<b>Odor threshold:</b>	Not determined.
<b>pH-value:</b>	Not applicable.
<b>Change in condition</b>	
<b>Melting point/Melting range:</b>	145-147 °C (293-297 °F)
<b>Boiling point/Boiling range:</b>	Not determined
<b>Sublimation temperature / start:</b>	Not determined
<b>Flash point:</b>	
<b>Flammability (solid, gaseous)</b>	Not determined.
<b>Ignition temperature:</b>	Not determined
<b>Decomposition temperature:</b>	Not determined
<b>Auto igniting:</b>	Not determined.
<b>Danger of explosion:</b>	
<b>Explosion limits:</b>	Product does not present an explosion hazard.
<b>Lower:</b>	Not determined
<b>Upper:</b>	Not determined
<b>Vapor pressure:</b>	Not applicable.
<b>Density:</b>	Not determined
<b>Relative density</b>	Not determined.
<b>Vapor density</b>	Not applicable.
<b>Evaporation rate</b>	Not applicable.
<b>Solubility in / Miscibility with</b>	
<b>Water:</b>	Not determined
<b>Partition coefficient (n-octanol/water):</b>	Not determined.
<b>Viscosity:</b>	
<b>dynamic:</b>	Not applicable.
<b>kinematic:</b>	Not applicable.
<b>Other information</b>	No further relevant information available.

**10 Stability and reactivity**

<b>Reactivity</b>	No information known.
<b>Chemical stability</b>	Stable under recommended storage conditions.
<b>Thermal decomposition / conditions to be avoided:</b>	Decomposition will not occur if used and stored according to specifications.
<b>Possibility of hazardous reactions</b>	No dangerous reactions known
<b>Conditions to avoid</b>	No further relevant information available.
<b>Incompatible materials:</b>	Oxidizing agents
<b>Hazardous decomposition products:</b>	
Carbon monoxide and carbon dioxide	
Nitrogen oxides	
Sulfur oxides (SOx)	
Hydrogen cyanide	

**11 Toxicological information**

<b>Information on toxicological effects</b>	
<b>Acute toxicity:</b>	
Harmful if inhaled.	
Harmful in contact with skin.	
Harmful if swallowed.	
Danger through skin absorption.	
<b>LD/LC50 values that are relevant for classification:</b>	No data
<b>Skin irritation or corrosion:</b>	Causes skin irritation.
<b>Eye irritation or corrosion:</b>	Causes serious eye irritation.
<b>Sensitization:</b>	No sensitizing effects known.
<b>Germ cell mutagenicity:</b>	No effects known.
<b>Carcinogenicity:</b>	No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
<b>Reproductive toxicity:</b>	No effects known.
<b>Specific target organ system toxicity - repeated exposure:</b>	No effects known.
<b>Specific target organ system toxicity - single exposure:</b>	May cause respiratory irritation.
<b>Aspiration hazard:</b>	No effects known.
<b>Subacute to chronic toxicity:</b>	No effects known.
<b>Subacute to chronic toxicity:</b>	
Nitriles may resemble cyanides in toxicity. Exposure to nitriles may cause increased salivation, flushing of the face, eye and respiratory tract irritation, shallow respiration, nausea, vomiting, weakness, headache and diarrhea. Jaundice, anemia, and leucocytosis has been reported in some cases.	
<b>Additional toxicological information:</b>	To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

**12 Ecological information**



<b>Toxicity</b>	
<b>Aquatic toxicity:</b>	No further relevant information available.
<b>Persistence and degradability</b>	No further relevant information available.
<b>Bioaccumulative potential</b>	No further relevant information available.
<b>Mobility in soil</b>	No further relevant information available.
<b>Additional ecological information:</b>	
<b>General notes:</b>	
Do not allow material to be released to the environment without proper governmental permits.	
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.	
Avoid transfer into the environment.	
<b>Results of PBT and vPvB assessment</b>	
<b>PBT:</b>	Not applicable.
<b>vPvB:</b>	Not applicable.
<b>Other adverse effects</b>	No further relevant information available.

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**13 Disposal considerations**  
**Waste treatment methods**  
**Recommendation** Consult state, local or national regulations to ensure proper disposal.  
**Uncleaned packagings:**  
**Recommendation:** Disposal must be made according to official regulations.

**14 Transport information**

UN-Number	UN3439
DOT, IMDG, IATA	
UN proper shipping name	Nitriles, solid, toxic, n.o.s. (p-Toluenesulfonylacetonitrile)
DOT	NITRILES, SOLID, TOXIC, N.O.S. (p-Toluenesulfonylacetonitrile)
IMDG, IATA	
Transport hazard class(es)	
DOT	
	
Class	6.1 Toxic substances.
Label	6.1
Class	6.1 (T2) Toxic substances
Label	6.1
IMDG, IATA	
	
Class	6.1 Toxic substances.
Label	6.1
Packing group	III
DOT, IMDG, IATA	
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Toxic substances
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT	
Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3439, Nitriles, solid, toxic, n.o.s. (p-Toluenesulfonylacetonitrile), 6.1, III

**15 Regulatory information**

**Safety, health and environmental regulations/legislation specific for the substance or mixture**  
**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)  
**Hazard pictograms**



GHS06

**Signal word** Danger

**Hazard statements**  
H302+H312 Harmful if swallowed or in contact with skin.  
H331 Toxic if inhaled.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H335 May cause respiratory irritation.

**Precautionary statements**  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P405 Store locked up.  
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**National regulations**  
This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.  
**SARA Section 313 (specific toxic chemical listings)** Substance is not listed.  
**California Proposition 65**  
**Prop 65 - Chemicals known to cause cancer** Substance is not listed.  
**Prop 65 - Developmental toxicity** Substance is not listed.  
**Prop 65 - Developmental toxicity, female** Substance is not listed.  
**Prop 65 - Developmental toxicity, male** Substance is not listed.  
**Information about limitation of use:** For use only by technically qualified individuals.  
**Other regulations, limitations and prohibitive regulations**  
**Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006.** Substance is not listed.  
**The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.**  
Substance is not listed.  
**Annex XIV of the REACH Regulations (requiring Authorisation for use)** Substance is not listed.  
**Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

**Product name:** *p-Toluenesulfonylacetonitrile*

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**16 Other information**

*Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.*

**Department issuing SDS:** Global Marketing Department  
**Date of preparation / last revision** 11/23/2015 / -  
**Abbreviations and acronyms:**  
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)  
IMDG: International Maritime Code for Dangerous Goods  
DOT: US Department of Transportation  
IATA: International Air Transport Association  
EINECS: European Inventory of Existing Commercial Chemical Substances  
CAS: Chemical Abstracts Service (division of the American Chemical Society)  
HMIS: Hazardous Materials Identification System (USA)  
WHMIS: Workplace Hazardous Materials Information System (Canada)  
LC50: Lethal concentration, 50 percent  
LD50: Lethal dose, 50 percent  
vPvB: very Persistent and very Bioaccumulative  
ACGIH: American Conference of Governmental Industrial Hygienists (USA)  
OSHA: Occupational Safety and Health Administration (USA)  
NTP: National Toxicology Program (USA)  
IARC: International Agency for Research on Cancer  
EPA: Environmental Protection Agency (USA)

USA