3-Pentenenitrile

sc-231896

Material Safety Data Sheet

Hazard Alert Code Key:	EXTREME	HIGH	MODERATE	LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
3-Pentenenitrile

STATEMENT OF HAZARDOUS NATURE
CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA

SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800

EMERGENCY
ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS
C5-H7-N, "nitrile, 3-pentene"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	3		
Toxicity:	3		
Body Contact:	2		
Reactivity:	2		
Chronic:	2		

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4

CANADIAN WHMIS SYMBOLS

EMERGENCY OVERVIEW

RISK
Toxic by inhalation.
Contact with acids liberates very toxic gas.
Irritating to eyes.
Harmful in contact with skin and if swallowed.
Flammable.
May cause long-term adverse effects in the environment.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED
■ Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage to the health of the individual.
■ Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide.
The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin.
■ Rats receiving a high oral doses of 2-pentenenitrile and its isomers showed hyperactivity, tremors and incoordination.
■ Cyanide poisoning can cause increased saliva output, nausea without vomiting, anxiety, confusion, vertigo, dizziness, stiffness of the lower jaw, convulsions, spasm, paralysis, coma and irregular heartbeat, and stimulation of breathing followed by failure.
Often the skin becomes cyanosed (blue-gray), and this is often delayed.

EYE
■ This material may produce eye irritation in some persons and produce eye damage 24 hours or more after instillation.
Moderate inflammation may be expected with redness; conjunctivitis may occur with prolonged exposure.
■ Eye contact with pentenitriles may produce tearing and blurred vision.

SKIN
■ Skin contact with the material may be harmful; systemic effects may resultfollowing absorption.
■ The liquid may be miscible with fats or oils and may degrease the skin, producing a skin reaction described as non-allergic contact dermatitis.
The material is unlikely to produce an irritant dermatitis as described in EC Directives .
■ A mixture of 2-pentenenitrile and its related isomers was moderately toxic by skin contact.
Effects of a high single dose included laboured breathing, dilated pupils, incoordination and tremors.
■ Open cuts, abraded or irritated skin should not be exposed to this material.
■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.
Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED
■ Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may produce toxic effects; these may be fatal.
■ The material is not thought to produce respiratory irritation (as classified using animal models).
Nevertheless inhalation of vapors, fumes or aerosols, especially for prolonged periods, may produce respiratory discomfort and occasionally, distress.
■ Rats exposed by inhalation for 4 hours to concentrations exceeding 100 ppm 2-pentenenitrile and its isomers showed hyperactivity, abnormal gait, posture and vocalisations with some effects observed up to 28 days following exposure.
No effects were observed at 8 ppm.
■ Inhalation hazard is increased at higher temperatures.

CHRONIC HEALTH EFFECTS
■ There has been some concern that this material can cause cancer or mutations but there is not enough data to make an assessment.
Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.
No genetic damage could be demonstrated in bacterial cells following exposure to 2-pentenenitrile and its isomers.
Chronic exposure to cyanides and certain nitriles may result in interference to iodine uptake by thyroid gland and its consequent enlargement. This occurs following metabolic conversion of the cyanide moiety to thiocyanate.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
3-pentenenitrile	4635-87-4	>98

Section 4 - FIRST AID MEASURES

SWALLOWED
· IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY. · Where Medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:

EYE
■ If this product comes in contact with the eyes: · Immediately hold eyelids apart and flush the eye continuously with running water. · Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN
■ If skin contact occurs: · Immediately remove all contaminated clothing, including footwear · Flush skin and hair with running water (and

soap if available).

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN

· Signs symptoms of acute cyanide poisoning reflect cellular hypoxia and are often non-specific.
· Cyanosis may be a late finding.

Section 5 - FIRE FIGHTING MEASURES

Vapor Pressure (mmHg):	24.752 (50 C)
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.837
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

· Foam.
· Dry chemical powder.

FIRE FIGHTING

· Alert Emergency Responders and tell them location and nature of hazard.
· Wear breathing apparatus plus protective gloves for fire only.
When any large container (including road and rail tankers) is involved in a fire,
consider evacuation by 1000 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

· Liquid and vapor are flammable.
· Moderate fire hazard when exposed to heat or flame.
Combustion products include: carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NOx), other pyrolysis products typical of burning organic material.
May emit poisonous fumes.
WARNING: Long standing in contact with air and light may result in the formation
of potentially explosive peroxides.

FIRE INCOMPATIBILITY

■ Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids,chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:
Safety Glasses.
Chemical goggles.
Gloves:
Respirator:
Type A-P Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS
■ Environmental hazard - contain spillage.
· Remove all ignition sources.
· Clean up all spills immediately.
MAJOR SPILLS
■ Environmental hazard - contain spillage.
· Clear area of personnel and move upwind.
· Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

■ The substance accumulates peroxides which may become hazardous only if it evaporates or is distilled or otherwise treated to concentrate the peroxides. The substance may concentrate around the container opening for example.
Purchases of peroxidisable chemicals should be restricted to ensure that the chemical is used completely before it can become peroxidised.
· A responsible person should maintain an inventory of peroxidisable chemicals or annotate the general chemical inventory to indicate which chemicals are subject to peroxidation. An expiration date should be determined. The chemical should either be treated to remove peroxides or disposed of before this date.
· The person or laboratory receiving the chemical should record a receipt date on the bottle. The individual opening the container should add an opening date.
· Unopened containers received from the supplier should be safe to store for 18 months.
· Opened containers should not be stored for more than 12 months.
· Avoid all personal contact, including inhalation.
· Wear protective clothing when risk of exposure occurs.
· Containers, even those that have been emptied, may contain explosive vapours.

· Do NOT cut, drill, grind, weld or perform similar operations on or near containers.

RECOMMENDED STORAGE METHODS

· Lined metal can, Lined metal pail/drum
· Plastic pail.
For low viscosity materials
· Drums and jerricans must be of the non-removable head type.
· Where a can is to be used as an inner package, the can must have a screwed enclosure.
All inner and sole packagings for substances that have been assigned to Packaging Groups I or II on the basis of inhalation toxicity criteria, must be hermetically sealed.

STORAGE REQUIREMENTS

· Store in original containers.
· Keep containers securely sealed.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

• 3-pentenenitrile: CAS:4635-87-4 CAS:16529-66-1

PERSONAL PROTECTION




RESPIRATOR

Type A-P Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE

· Safety glasses with side shields.
· Chemical goggles.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.
Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:
· frequency and duration of contact,
· chemical resistance of glove material,
· glove thickness and
· dexterity
Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).
· When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
· When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
· Contaminated gloves should be replaced.
Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.
· Neoprene rubber gloves.

OTHER

· Overalls.
· Eyewash unit.
· Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity.
· For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets), non sparking safety footwear.
Neoprene whole body suit, neoprene boots, apron. Dispose of saturated clothing.

ENGINEERING CONTROLS

■ Local exhaust ventilation usually required. If risk of overexposure exists, wear an approved respirator.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Does not mix with water.
Floats on water.
Toxic or noxious vapours/gas.

Contact with acids liberates very toxic gas.

State	LIQUID	Molecular Weight	81.12
Melting Range (°F)	Not available	Viscosity	Not Available
Boiling Range (°F)	291- 297	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	104	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapor Pressure (mmHg)	24.752 (50 C)
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	0.837
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	2.8
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE
Colourless liquid with pungent odour; does not mix well with water (7.5 g/l, 25 C).

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY
· Presence of incompatible materials.
· Product is considered stable.

STORAGE INCOMPATIBILITY
■ For 2-pentenenitrile:
· Prior to distilling this material treat to remove any peroxides.
· Distillation should be performed under atmospheric pressure where residual peroxides are thermally destroyed whilst still diluted.
· Low temperature vacuum distillation may allow potentially dangerous residual peroxides to concentrate.
· Nitriles may polymerize in the presence of metals and some metal compounds.
· They are incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions.
· The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable.
· The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation.
· Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds.
BRETHERICK L.: Handbook of Reactive Chemical Hazards.
· Avoid strong acids, bases.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

3-pentenenitrile

TOXICITY AND IRRITATION
3-PENTENENITRILE:
■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

TOXICITY	IRRITATION
Inhalation (Rat) LC50: 420 ppm/4h *	Nil Reported

■ The pentenenitriles are composed of linear straight and branched chain alkenes with a common functional group, nitrile, at one end of the parent alkene chain. This category 2 is composed of individual isomers containing five carbon atoms that differ by the position of a carbon to carbon double bond relative to the nitrile group. These substances are produced in the production of adiponitrile.
The acute data that exists for these chemicals indicate that the chemicals produce similar toxicity profiles rat oral values for ALD (approximate lethal dose) range from 300-2250 mg/kg. Inhalation LC50 values 94 hours,) for rat range from 420 ppm to 3000 ppm making them moderately-toxic by inhalation. Dermal toxicity is moderate to high.
Pentenenitriles are mild eye irritants but do not irritate the skin. They do not appear to be skin sensitisers.
The material may produce moderate eye irritation leading to inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.
Tremor, change in motor activity, ataxia recorded.

Section 12 - ECOLOGICAL INFORMATION

May cause long-term adverse effects in the environment.
This material and its container must be disposed of as hazardous waste.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
3-pentenenitrile	LOW		LOW	HIGH

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information
Ignitability characteristic: use EPA hazardous waste number D001 (waste code I)
Reactivity characteristic: use EPA hazardous waste number D003 (waste code R).

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.
¦ Puncture containers to prevent re-use and bury at an authorized landfill.
Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.
A Hierarchy of Controls seems to be common - the user should investigate:
· Reduction
· Reuse
· Recycling
· Disposal (if all else fails)
This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.
DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.
· Recycle wherever possible.
· Consult manufacturer for recycling options or consult Waste Management Authority for disposal if no suitable treatment or disposal facility can be identified.

Section 14 - TRANSPORTATION INFORMATION

DOT:
Symbols: None Hazard class or Division: 6.1
Identification Numbers: UN3275 PG: II
Label Codes: 6.1, 3 Special provisions: IB2, T11,
TP2, TP13,
TP27
Packaging: Exceptions: 153 Packaging: Non- bulk: 202
Packaging: Exceptions: 153 Quantity limitations: 5 L
Passenger aircraft/rail:
Quantity Limitations: Cargo 60 L Vessel stowage: Location: B
aircraft only:
Vessel stowage: Other: 40, 52
Hazardous materials descriptions and proper shipping names:
Nitriles, toxic, flammable, n.o.s.

Air Transport IATA:

ICAO/IATA Class: 6.1 (3) ICAO/IATA Subrisk: None
UN/ID Number: 3275 Packing Group: II
Special provisions: A4
Cargo Only
Packing Instructions: 60 L Maximum Qty/Pack: 5 L
Passenger and Cargo Passenger and Cargo
Packing Instructions: 662 Maximum Qty/Pack: 654
Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity
Packing Instructions: 1 L Maximum Qty/Pack: Y641
Shipping Name: NITRILES, TOXIC, FLAMMABLE, N.O.S. *
(CONTAINS 3-PENTENENITRILE)

Maritime Transport IMDG:

IMDG Class: 6.1 IMDG Subrisk: 3
UN Number: 3275 Packing Group: II
EMS Number: F-E , S-D Special provisions: 274
Limited Quantities: 100 ml
Shipping Name: NITRILES, TOXIC, FLAMMABLE, N.O.S.
(contains 3-pentenenitrile)

Section 15 - REGULATORY INFORMATION

3-pentenenitrile (CAS: 4635-87-4,16529-66-1) is found on the following regulatory lists;
"Canada Non-Domestic Substances List (NDSL)","OECD Representative List of High Production Volume (HPV) Chemicals","US EPA High Production Volume Program Chemical List","US Toxic Substances Control Act (TSCA) - Inventory"

Section 16 - OTHER INFORMATION

Ingredients with multiple CAS Nos
Ingredient Name CAS 3-pentenenitrile 4635-87-4, 16529-66-1

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■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.
A list of reference resources used to assist the committee may be found at:
www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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