

# 4-Nitrothiophenol

sc-232931

Material Safety Data Sheet



The Power is Question

Hazard Alert Code Key:

EXTREME

HIGH

MODERATE

LOW

## Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

### PRODUCT NAME

4-Nitrothiophenol

### 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

### PRODUCT USE

Intermediate.

### SYNONYMS

C6-H5-N-O2-S, "benzenethiol, p-nitro-", "benzenethiol, 4-nitro-", p-nitrobenzenethiol, 4-nitrobenzenethiol, "p-nitrophenyl mercaptan", p-nitrothiophenol

## Section 2 - HAZARDS IDENTIFICATION

### CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	2		
Reactivity:	2		
Chronic:	2		

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



### CANADIAN WHMIS SYMBOLS



## EMERGENCY OVERVIEW

### RISK

Irritating to eyes, respiratory system and skin.

### POTENTIAL HEALTH EFFECTS

#### ACUTE HEALTH EFFECTS

#### SWALLOWED

- Accidental ingestion of the material may be damaging to the health of the individual.
- The substance and/or its metabolites may bind to hemoglobin inhibiting normal uptake of oxygen. This condition, known as "methemoglobinemia", is a form of oxygen starvation (anoxia).

#### EYE

- This material can cause eye irritation and damage in some persons.

#### SKIN

- This material can cause inflammation of the skin on contact in some persons.
- The material may accentuate any pre-existing dermatitis condition.
- Skin contact is not thought to have harmful health effects, however the material may still produce health damage following entry through wounds, lesions or abrasions.
- 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

- The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Inhalation of dusts, generated by the material during the course of normal handling, may be damaging to the health of the individual.
- Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.
- Thiols (particularly ethyl mercaptan) produce lethargy or sleepiness. Exposure to high levels may result in nausea, vomiting, restlessness, muscle incoordination and or paralysis, bluing of skin, depression of breathing, coma and death.

#### CHRONIC HEALTH EFFECTS

- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems. Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems. Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Chronic exposure to mercaptans may result in damage to the lungs, kidneys and liver.

## Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
4-nitrothiophenol	1849-36-1	>98

## Section 4 - FIRST AID MEASURES

#### SWALLOWED

· If swallowed do NOT induce vomiting. · If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

#### EYE

■ If this product comes in contact with the eyes: · Wash out immediately with fresh 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

■ Symptoms of vasodilation and reflex tachycardia may present following organic nitrate overdose; most organic nitrates are extensively metabolized by hydrolysis to inorganic nitrites. Organic nitrates and nitrites are readily absorbed through the skin, lungs, mucosa and gastrointestinal tract.

The toxicity of nitrates and nitrites result from their vasodilating properties and their propensity to form methemoglobin.

- Most produce a peak effect within 30 minutes.
- Clinical signs of cyanosis appear before other symptoms because of the dark pigmentation of methemoglobin.

## Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Negligible
Upper Explosive Limit (%):	Not available.
Specific Gravity (water=1):	Not available
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.
- When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 100 metres in all directions.

### GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Combustible solid which burns but propagates flame with difficulty.
  - Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust may burn rapidly and fiercely if ignited.
- Combustion products include: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), sulfur oxides (SO<sub>x</sub>), other pyrolysis products typical of burning organic material.
- The dry lithium salt of 4-nitrothiophenol may detonate on exposure to air.

### FIRE INCOMPATIBILITY

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

### PERSONAL PROTECTION

Glasses:  
Chemical goggles.  
Gloves:  
Respirator:  
Particulate

## Section 6 - ACCIDENTAL RELEASE MEASURES

### MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.
- Use dry clean up procedures and avoid generating dust.
- Place in a suitable, labelled container for waste disposal.

WARNING: Never use dry, powdered hypochlorite or other strong oxidizer for mercaptan spills, as autoignition can occur.

### MAJOR SPILLS

- Moderate hazard.
- CAUTION: Advise personnel in area.
- Alert Emergency Responders and tell them location and nature of hazard.

## Section 7 - HANDLING AND STORAGE

### PROCEDURE FOR HANDLING

- The careful design and assembly of equipment is paramount to the control of mercaptan odors. Although careful planning reduces the chances for leaks developing in the system, it is important to be prepared to locate and stop small leaks promptly. It is recommended that a leak check be made prior to every run carried out under pressure in metal equipment with a mercaptan or hydrogen sulfide present.

An effective method to obtain a leak-free system involves two steps:

- Charge the system with nitrogen gas or other inert, nontoxic gas to a pressure at least as high as will be used in practice, and check for a drop in pressure with time on a suitable gauge. In some cases, it is advantageous to block off sections of the system to facilitate finding the leak. If any leaks are detected by using a foaming detergent solution, correct them and recheck.
- Recharge the system with hydrogen sulfide gas. Since hydrogen sulfide is very toxic, it is good practice to charge the system in steps of increasing pressure, until it is certain that no large leaks are present. Any remaining small leaks can be located quickly by examining the system with lead acetate paper. Dilution of the hydrogen sulfide with nitrogen can also be considered.

To control odors in mercaptan reactions in the laboratory. All reactions must be carried out in a hood or, in the case of pressure reactions, in a closed in area equipped with an efficient exhaust fan. In the laboratory, the two basic types of reactions used are batch and continuous. Batch-type reactions at atmospheric pressure are generally conducted in glass equipment. If no significant quantity of a volatile mercaptan is present, the reaction can be carried out in a hood equipped with a charcoal bed in the exhaust line to absorb the mercaptan. In reactions

where appreciable quantities of a volatile mercaptan are present, a vent gas line can be connected to two caustic scrubbers in series, with an empty trap inserted between the reaction and scrubbers to avoid reverse flow of caustic into the reaction. Continuous-type reactions often include a continuous flow of volatile C1 to C4 mercaptans. In this case, the vented gases can be fed to an outside gas burner and stack for destruction of the odor by combustion.

A hood, equipped with a charcoal filter in the exhaust line, and a high linear air velocity (100 ft./min., minimum) is necessary for mercaptan reactions carried out in glass and certain small-scale reactions with stainless-steel. In reactions where relatively small amounts of mercaptans can escape, the charcoal bed can absorb the mercaptans and prevent the escape of odor to the outside atmosphere. However, in reactions with hydrogen sulfide or lower molecular weight mercaptans, e.g., C1-C4 mercaptans, the quantity of effluent gases is directed to an outside gas burner to convert the odorous compounds to acceptable combustion products, including CO<sub>2</sub> and SO<sub>2</sub>.

A very familiar and successful method for containing the odors of mercaptan (primarily C1 and C6) in laboratory reactions and distillations is to connect the condenser vent to two caustic scrubbers in series with an empty trap between the system and the scrubbers to catch the caustic in the event of reverse flow. Gas bubblers fitted with sintered-glass dip tubes and charged with aqueous sodium hydroxide (5 to 20%) are commonly used. Frequently, a low flow of inert gas, e.g., nitrogen, is used to maintain a steady flow through the bubbler.

Sodium hypochlorite solution (3-10%) destroys the odor by converting the mercaptan predominantly to the corresponding sulfonic acid (sodium salt). A wash bottle with hypochlorite solution is very convenient for quickly eliminating or controlling the odor from small spills or when cleaning up glass equipment. A bath of this solution is also very useful. WARNING! Do not add this solution to a large quantity of concentrated mercaptan, since a violent reaction may occur.

A 30-40% aqueous solution of lead acetate trihydrate serves as a detector for methyl and ethyl mercaptan as well as hydrogen sulfide. A wash bottle of lead acetate solution is used to moisten a piece of filter paper or paper towel which is then held close to (no contact) the suspected leak. With hydrogen sulfide the paper turns black and with the two mercaptans a yellow color is obtained (high sensitivity).

A large plastic bag should be kept in the hood, to store any odorous waste materials. The plastic bags can then be sealed in fiber drums for disposal. Glass bottles containing mercaptans and other odorous compounds can also be packed in fiber drums for odor-containment and properly marked for disposal.

A box of disposable gloves should be available, and the gloves should be discarded (in plastic bag in hood) after each use. Disposable aprons or lab coats are recommended, since clothing contacted with mercaptan is often difficult to deodorise.

Types of tubing found useful with mercaptans include: Teflon<sup>®</sup>, TFE, FEP, and PFA, Bev-a-line (IV or V), and 316 stainless steel. Bev-a-line tubing has a polyethylene liner cross-linked to an ethylene vinyl acetate shell, a useful temperature range of -60 C to +250 C, and is heat bondable. It is less expensive than TFE tubing and is convenient for flexible connections between glass and metal tubing lines. It is available from most laboratory supply houses. Copper and brass are unacceptable materials for handling mercaptans, because mercaptans are H<sub>2</sub>S are highly corrosive to copper and brass. Care should be taken not to use valves and gauges with brass components.

Atofina Chemicals.

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

- Do NOT cut, drill, grind or weld such containers.
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

## RECOMMENDED STORAGE METHODS

- Polyethylene or polypropylene container.
- Check all containers are clearly labelled and free from leaks.

## STORAGE REQUIREMENTS

- Observe manufacturer's storing and handling recommendations.

## Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

### EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m <sup>3</sup>	STEL ppm	STEL mg/m <sup>3</sup>	Peak ppm	Peak mg/m <sup>3</sup>	TWA F/CC	Notes
Canada - British Columbia Occupational Exposure Limits	4-nitrothiophenol (Particulates Insoluble or Poorly Soluble) Not Otherwise Classified (PNOC))		10 (N)						
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	4-nitrothiophenol (Particulates not otherwise regulated (PNOR)(f)-Respirable fraction)		5						
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	4-nitrothiophenol (Particulates not otherwise regulated Respirable fraction)		5						

US - California Permissible Exposure Limits for Chemical Contaminants	4-nitrothiophenol (Particulates not otherwise regulated Respirable fraction)	5	(n)
US - Oregon Permissible Exposure Limits (Z-1)	4-nitrothiophenol (Particulates not otherwise regulated - (PNOR) (f) Total Dust)	10	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means “particles not otherwise regulated.”
US - Michigan Exposure Limits for Air Contaminants	4-nitrothiophenol (Particulates not otherwise regulated, Respirable dust)	5	
Canada - Prince Edward Island Occupational Exposure Limits	4-nitrothiophenol (Particles (Insoluble or Poorly Soluble) [NOS] Inhalable particles)	10	See Appendix B current TLV/BEI Book
US - Oregon Permissible Exposure Limits (Z-1)	4-nitrothiophenol (Particulates not otherwise regulated - (PNOR) (f) Respirable Fraction)	5	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means “particles not otherwise regulated.”

## ENDOELTABLE

### PERSONAL PROTECTION



### RESPIRATOR

Particulate

Consult your EHS staff for recommendations

### EYE

- Safety glasses with side shields.
- Chemical goggles.

### HANDS/FEET

■ 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.

Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.

- polychloroprene
- nitrile rubber
- butyl rubber
- fluorocautchouc
- polyvinyl chloride

Gloves should be examined for wear and/ or degradation constantly.

#### OTHER

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.
- Eye wash unit.

#### ENGINEERING CONTROLS

· Local exhaust ventilation is required where solids are handled as powders or crystals; even when particulates are relatively large, a certain proportion will be powdered by mutual friction.

· Exhaust ventilation should be designed to prevent accumulation and recirculation of particulates in the workplace.

## Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

### PHYSICAL PROPERTIES

Solid.

Does not mix with water.

State	Divided solid	Molecular Weight	155.18
Melting Range (°F)	165.2- 170.6	Viscosity	Not Applicable
Boiling Range (°F)	Not available	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	Not available	pH (1% solution)	Not available
Decomposition Temp (°F)	Not available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available.	Vapour Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	Not available
Lower Explosive Limit (%)	Not available.	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Negligible	Evaporation Rate	Not applicable

### APPEARANCE

Gold-orange to yellow powder with unpleasant odour; does not mix well with water.

## Section 10 - CHEMICAL STABILITY

### CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

### STORAGE INCOMPATIBILITY

· Nitroaromatic and in particular polynitroaromatic compounds may present a severe explosion risk if subjected to shock or heated rapidly and uncontrollably as in fire situations.

· In addition, when such compounds are heated more moderately with caustic alkalies, even when water or organic solvents are present, there is also a risk of violent decomposition or explosion - several industrial accidents, which probably were due to such interactions, have occurred; this potential hazard often remains unacknowledged.

· Aromatic nitro compounds range from slight to strong oxidizing agents. If mixed with reducing agents, including hydrides, sulfides and nitrides, they may begin a vigorous reaction that culminates in a detonation. The explosive tendencies of aromatic nitro compounds are increased by the presence of multiple nitro groups.

· A range of exothermic decomposition energies for nitro compounds is given as 220-410 kJ/mol. The relationship between energy of decomposition and processing hazards has been the subject of discussion; it is suggested that values of energy released per unit of mass, rather than on a molar basis (J/g) be used in the assessment. For example, in "open vessel processes" (with man-hole size openings, in an industrial setting), substances with exothermic decomposition energies below 500 J/g are unlikely to present a danger, whilst those in "closed vessel processes" (opening is a safety valve or bursting disk) present some danger where the decomposition energy exceeds 150 J/g.

BRETHERRICK: Handbook of Reactive Chemical Hazards, 4th Edition.

Avoid reaction with oxidizing agents, bases and strong reducing agents.

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

## Section 11 - TOXICOLOGICAL INFORMATION

4-nitrothiophenol

### TOXICITY AND IRRITATION

#### 4-NITROTHIOPHENOL:

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.  
■ Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

No significant acute toxicological data identified in literature search.

## Section 12 - ECOLOGICAL INFORMATION

This material and its container must be disposed of as hazardous waste.

### Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
4-nitrothiophenol	HIGH		LOW	MED

## Section 13 - DISPOSAL CONSIDERATIONS

### Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

! 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. 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: A G Hazard class or Division: 9

Identification Numbers: UN3335 PG: None

Label Codes: 9 Special provisions: A35

Packaging: Exceptions: 155 Packaging: Non- bulk: 204

Packaging: Exceptions: 155 Quantity limitations: No limit

Passenger aircraft/rail:

Quantity Limitations: Cargo No limit Vessel stowage: Location: A aircraft only:

Vessel stowage: Other: None

Hazardous materials descriptions and proper shipping names:

Aviation regulated solid, n.o.s.

### Air Transport IATA:

ICAO/IATA Class: 9 ICAO/IATA Subrisk: None

UN/ID Number: 3335 Packing Group: -

Special provisions: A27

Cargo Only

Packing Instructions: 200 kg Maximum Qty/Pack: 100 kg

Passenger and Cargo Passenger and Cargo

Packing Instructions: 906 Maximum Qty/Pack: 906

Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity

Packing Instructions: Forbidden Maximum Qty/Pack: Forbidden

Shipping Name: AVIATION REGULATED SOLID, N.O.S. \*

†(CONTAINS 4-NITROTHIOPHENOL)  
NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: IMDG

## Section 15 - REGULATORY INFORMATION

### **4-nitrothiophenol (CAS: 1849-36-1) is found on the following regulatory lists;**

"Canada - British Columbia Occupational Exposure Limits", "Canada - Prince Edward Island Occupational Exposure Limits", "Canada National Pollutant Release Inventory (NPRI)", "US - California Permissible Exposure Limits for Chemical Contaminants", "US - Michigan Exposure Limits for Air Contaminants", "US - Oregon Permissible Exposure Limits (Z-1)", "US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants", "US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants"

## Section 16 - OTHER INFORMATION

*Reasonable care has been taken in the preparation of this information, but the author makes no warranty of merchantability or any other warranty, expressed or implied, with respect to this information. The author makes no representations and assumes no liability for any direct, incidental or consequential damages resulting from its use. For additional technical information please call our toxicology department on +800 CHEMCALL.*

■ 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](http://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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