

# Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
	Harmful compound, minimize exposure. Irritating to skin, eyes, and the respiratory system. <b>POSSIBLE MUTAGEN. MINIMIZE EXPOSURE.</b> This material is harmful to aquatic organisms and may cause long term adverse effects to the aquatic environment.	

## Section I. Chemical Product and Company Identification

Chemical Name	<b>3-Nitrobenzoic Acid</b>		
Catalog Number	N0154	Supplier	TCI America 9211 N. Harborsgate St. Portland OR 1-800-423-8616
Synonym	Benzoic acid, 3-nitro- (CA INDEX NAME); m-Nitrobenzenecarboxylic Acid		
Chemical Formula	C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub>		
CAS Number	121-92-6	In case of Emergency Call	<b>Chemtrec®</b> <b>(800) 424-9300 (U.S.)</b> <b>(703) 527-3887 (International)</b>

## Section II. Composition and Information on Ingredients

Chemical Name	CAS Number	Percent (%)	TLV/PEL	Toxicology Data
3-Nitrobenzoic Acid	121-92-6	Min. 99.0 (GC,T)	This compound is classified as a possible mutagen. There is no acceptable exposure limit for a mutagen.	Mouse LD <sub>50</sub> (oral) 1450 mg/kg Mouse LD <sub>50</sub> (intraperitoneal) 610 mg/kg Mouse LD <sub>50</sub> (intravenous) 640 mg/kg

## Section III. Hazards Identification

Acute Health Effects	Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.
Chronic Health Effects	<b>CARCINOGENIC EFFECTS</b> : Not available. <b>MUTAGENIC EFFECTS</b> : Not available. <b>TERATOGENIC EFFECTS</b> : Not available. <b>DEVELOPMENTAL TOXICITY</b> : Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

## Section IV. First Aid Measures

Eye Contact	Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.
Skin Contact	In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.
Inhalation	If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.
Ingestion	INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive.

## Section V. Fire and Explosion Data

Flammability	May be combustible at high temperature.	Auto-Ignition	480 °C (896 °F)
Flash Points	190 °C (374 °F).	Flammable Limits	Not available.
Combustion Products	These products are toxic carbon oxides (CO, CO <sub>2</sub> ), nitrogen oxides (NO, NO <sub>2</sub> ).		
Fire Hazards	Not available.		
Explosion Hazards	Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.		
Fire Fighting Media and Instructions	SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet. Consult with local fire authorities before attempting large scale fire-fighting operations.		

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Emergency phone number (800) 424-9300

**Section VI. Accidental Release Measures**

Spill Cleanup Instructions Harmful material. Irritating material. Possibly mutagenic material. Use a shovel to put the material into a convenient waste disposal container. Finish cleaning the spill by rinsing any contaminated surfaces with copious amounts of water. Consult federal, state, and/or local authorities for assistance on disposal.

**Section VII. Handling and Storage**

Handling and Storage Information HARMFUL. IRRITANT. POSSIBLE MUTAGEN. Keep away from heat. Mechanical exhaust required. When not in use, tightly seal the container and store in a dry, cool place. Avoid excessive heat and light. Do not breathe dust. Always store away from incompatible compounds such as oxidizing agents, reducing agents, alkalis (bases).

**Section VIII. Exposure Controls/Personal Protection**

Engineering Controls Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection Splash goggles. Lab coat. Dust respirator. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product. Be sure to use a MSHA/NIOSH approved respirator or equivalent.



Exposure Limits This compound is classified as a possible mutagen. There is no acceptable exposure limit for a mutagen.

**Section IX. Physical and Chemical Properties**

Physical state @ 20°C	Solid. (Pale yellow, crystal ~ powder.)	Solubility	Not available.
Specific Gravity	1.49 (water=1)		
Molecular Weight	167.12	Partition Coefficient	Log P <sub>ow</sub> : 1.82
Boiling Point	Not available.	Vapor Pressure	Not applicable.
Melting Point	142°C (287.6°F)	Vapor Density	Not available.
Refractive Index	Not available.	Volatility	Not available.
Critical Temperature	Not available.	Odor	Not available.
Viscosity	Not available.	Taste	Not available.

**Section X. Stability and Reactivity Data**

Stability This material is stable if stored under proper conditions. (See Section VII for instructions)

Conditions of Instability Avoid excessive heat and light.

Incompatibilities Reactive with strong oxidizing agents, strong reducing agents, strong alkalis (bases).

**Section XI. Toxicological Information**

RTECS Number DH5000000

Routes of Exposure Eye Contact. Ingestion. Inhalation.

Toxicity Data  
 Mouse LD<sub>50</sub> (oral) 1450 mg/kg  
 Mouse LD<sub>50</sub> (intraperitoneal) 610 mg/kg  
 Mouse LD<sub>50</sub> (intravenous) 640 mg/kg

Chronic Toxic Effects  
**CARCINOGENIC EFFECTS** : Not available.  
**MUTAGENIC EFFECTS** : Not available.  
**TERATOGENIC EFFECTS** : Not available.  
**DEVELOPMENTAL TOXICITY**: Not available.  
 Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Acute Toxic Effects  
 Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.  
 Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

**Section XII. Ecological Information**

Ecotoxicity Not available.

Environmental Fate 3-Nitrobenzoic acid's production and use as a dye intermediate, reagent for alkaloids and thorium, and in the preparation of 5-amino-2-hydroxy benzoic acid may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of  $3.7 \times 10^{-5}$  mm Hg at 25 deg C indicates 3-nitrobenzoic acid will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase 3-nitrobenzoic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 26 days. Particulate-phase 3-nitrobenzoic acid will be removed from the atmosphere by wet or dry deposition. 3-Nitrobenzoic acid contains chromophores that absorb at wavelengths  $>290$  nm and therefore may be susceptible to direct photolysis by sunlight. If released to soil, 3-nitrobenzoic acid is expected to have moderate mobility based upon an estimated Koc of 240. The pKa of 3-nitrobenzoic acid is 3.46, indicating that this compound will exist almost entirely in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of  $3.8 \times 10^{-10}$  atm-cu m/mole. Biodegradation in soil is expected to be a slow environmental fate process. Decomposition of nitrobenzoic acid by soil microflora took greater than 64 days, and the compound did not degrade in soil after 25 days. If released into water, 3-nitrobenzoic acid is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Biodegradation of 3-nitrobenzoic acid is expected to occur in water based upon a 42.0% of theoretical BOD in river water after 5 days. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. A pKa of 3.46 indicates 3-nitrobenzoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore, volatilization from water surfaces is not expected to be an important fate process. An estimated BCF of 3.2 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to 3-nitrobenzoic acid may occur through dermal contact with this compound at workplaces where 3-nitrobenzoic acid is produced or used.

**Section XIII. Disposal Considerations**

Waste Disposal Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.

**Section XIV. Transport Information**

DOT Classification Not a DOT controlled material (United States).

PIN Number Not applicable.

Proper Shipping Name Not applicable.

Packing Group (PG) Not applicable.

DOT Pictograms

**Section XV. Other Regulatory Information and Pictograms**

TSCA Chemical Inventory (EPA) This compound is **ON** the EPA Toxic Substances Control Act (TSCA) inventory list.

WHMIS Classification (Canada) On DSL

EINECS Number (EEC) 204-508-5

EEC Risk Statements R20/21/22- Harmful by inhalation, in contact with skin and if swallowed.  
R36/37/38- Irritating to eyes, respiratory system and skin.  
R52- Harmful to aquatic organisms.

Japanese Regulatory Data ENCS No. 3-1505

**Section XVI. Other Information**

**Version 1.0**  
**Validated on 8/5/2011.**  
**Printed 8/5/2011.**

**Notice to Reader**

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local regulations.