

N α -(2,4-Dinitro-5-fluorophenyl)-L-alaninamide

sc-253171



The Power to Question

Material Safety Data Sheet

Hazard Alert Code
Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

N α -(2,4-Dinitro-5-fluorophenyl)-L-alaninamide

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

Company: Santa Cruz Biotechnology, Inc.

Address:

2145 Delaware Ave

Santa Cruz, CA 95060

Telephone: 800.457.3801 or 831.457.3800

Emergency Tel: CHEMWATCH: From within the US and

Canada: 877-715-9305

Emergency Tel: From outside the US and Canada: +800 2436

2255 (1-800-CHEMCALL) or call +613 9573 3112

PRODUCT USE

Chiral reagent for the assay of enantiomeric purity of amino-acids with HPLC.. For the derivatisation and resolution of amino-acids. Derivatised D- and L-amino acids can be resolved and quantitated by HPLC.

SYNONYMS

C9-H9-F-N4-O5, FC6H2(NO2)2NHCH(CH3)CONH2, FDAA, "Marfey' s Reagent"

Section 2 - HAZARDS IDENTIFICATION

CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Irritating to eyes, respiratory system and skin.

Harmful to aquatic organisms.

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).

Symptoms include cyanosis (a bluish discoloration skin and mucous membranes) and breathing difficulties. Symptoms may not be evident until several hours after exposure.

At about 15% concentration of blood methemoglobin there is observable cyanosis of the lips, nose and earlobes. Symptoms may be absent although euphoria, flushed face and headache are commonly experienced. At 25-40%, cyanosis is marked but little disability occurs other than that produced on physical exertion. At 40-60%, symptoms include weakness, dizziness, lightheadedness, increasingly severe headache, ataxia, rapid shallow respiration, drowsiness, nausea, vomiting, confusion, lethargy and stupor. Above 60% symptoms include dyspnea, respiratory depression, tachycardia or bradycardia, and convulsions. Levels exceeding 70% may be fatal.

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.
- 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.

CHRONIC HEALTH EFFECTS

- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

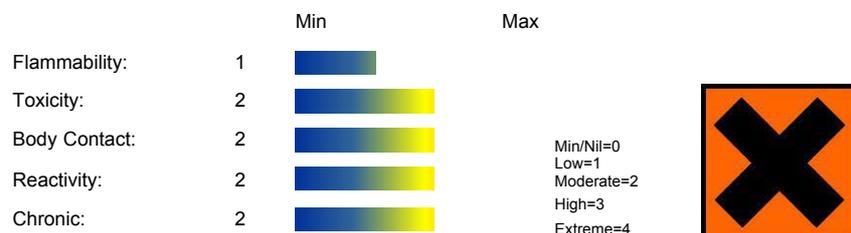
Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

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. Prime symptom is breathlessness; lung shadows show on X-ray.

Most arylamines are powerful poisons to the blood-making system. High chronic doses cause congestion of the spleen and tumor formation.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

HAZARD RATINGS



NAME	CAS RN	%
Nalpha-(2,4-dinitro-5-fluorophenyl)-L-alaninamide	95713-52-3	>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.
- Observe the patient carefully.
- Never give liquid to a person showing signs of being sleepy or with reduced awareness; i.e. becoming unconscious.
- Give water to rinse out mouth, then provide liquid slowly and as much as casualty can comfortably drink.
- Seek medical advice.

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.
 - If pain persists or recurs seek medical attention.
 - Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

SKIN

- If skin contact occurs:
 - Immediately remove all contaminated clothing, including footwear
 - Flush skin and hair with running water (and soap if available).
 - Seek medical attention in event of irritation.

INHALED

- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.
- Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
- Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.
- Transport to hospital, or doctor, without delay.

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 gastro-intestinal 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.
- Initial attention should be directed towards improving oxygen delivery, with assisted ventilation, if necessary. Hyperbaric oxygen has not demonstrated conclusive benefits.
- Institute cardiac monitoring, especially in patients with coronary artery or pulmonary disease.

- Hypotension should respond to Trendelenburg's position and intravenous fluids; otherwise dopamine may be needed.
- Naloxone, glucose and thiamine should be given if a multiple ingestion is suspected.
- Decontaminate using Ipecac Syrup for alert patients or lavage for obtunded patients who present within 2-4 hours of ingestion.
- Symptomatic patients with methemoglobin levels over 30% should receive methylene blue. (Cyanosis alone, is not an indication for treatment). The usual dose is 1-2 mg/kg of a 1% solution (10 mg/ml) IV over 5 minutes; repeat, using the same dose if symptoms of hypoxia fail to subside within 1 hour.

[Ellenhorn and Barceloux: Medical Toxicology] BIOLOGICAL EXPOSURE INDEX - BEI

These represent the determinants observed in specimens collected from a healthy worker who has been exposed at the Exposure Standard (ES or TLV):

Determinant	Index	Sampling Time	Comments
1. Methemoglobin in blood	1.5% of hemoglobin	During or end of shift	B,NS,SQ

B: Background levels occur in specimens collected from subjects NOT exposed

NS: Non-specific determinant; also observed after exposure to other materials

SQ: Semi-quantitative determinant - Interpretation may be ambiguous; should be used as a screening test or confirmatory test.

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.
- BCF (where regulations permit).
- Carbon dioxide.
- Water spray or fog - Large fires only.

FIRE FIGHTING

-
- Alert Emergency Responders and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.
- Prevent, by any means available, spillage from entering drains or water course.
- Use water delivered as a fine spray to control fire and cool adjacent area.
- DO NOT approach containers suspected to be hot.
- Cool fire exposed containers with water spray from a protected location.
- If safe to do so, remove containers from path of fire.
- Equipment should be thoroughly decontaminated after use.

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.
- Dry dust can be charged electrostatically by turbulence, pneumatic transport, pouring, in exhaust ducts and during transport.
- Build-up of electrostatic charge may be prevented by bonding and grounding.
- Powder handling equipment such as dust collectors, dryers and mills may require additional protection measures such as explosion venting.

Combustion products include: carbon monoxide (CO), carbon dioxide (CO₂), hydrogen fluoride, nitrogen oxides (NO_x), other pyrolysis products typical of burning organic material.

May emit poisonous fumes.

May emit corrosive fumes.

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.

MAJOR SPILLS

-
- Moderate hazard.
- CAUTION: Advise personnel in area.
- Alert Emergency Responders and tell them location and nature of hazard.
- Control personal contact by wearing protective clothing.
- Prevent, by any means available, spillage from entering drains or water courses.
- Recover product wherever possible.
- IF DRY: Use dry clean up procedures and avoid generating dust. Collect residues and place in sealed plastic bags or other

- containers for disposal. IF WET: Vacuum/shovel up and place in labelled containers for disposal.
- ALWAYS: Wash area down with large amounts of water and prevent runoff into drains.
- If contamination of drains or waterways occurs, advise emergency services.

ACUTE EXPOSURE GUIDELINE LEVELS (AEGL) (in ppm)

AEGL 1: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL 2: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL 3: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.
- DO NOT enter confined spaces until atmosphere has been checked.
- DO NOT allow material to contact humans, exposed food or food utensils.
- Avoid contact with incompatible materials.
- When handling, DO NOT eat, drink or smoke.
- Keep containers securely sealed when not in use.
- Avoid physical damage to containers.
- Always wash hands with soap and water after handling.
- Work clothes should be laundered separately.
- Launder contaminated clothing before re-use.
- Use good occupational work practice.
- Observe manufacturer's storing and handling recommendations.
- Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.

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.

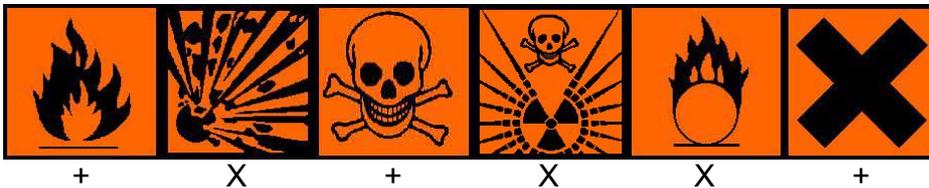
RECOMMENDED STORAGE METHODS

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

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

SAFE STORAGE WITH OTHER CLASSIFIED CHEMICALS



X: Must not be stored together

O: May be stored together with specific preventions

+: May be stored together

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m ³	STEL ppm	STEL mg/m ³	Peak ppm	Peak mg/m ³	TWA F/CC	Notes
US - Oregon Permissible Exposure Limits (Z3)	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Inert or Nuisance Dust: (d) Total dust)		10						*
US OSHA Permissible Exposure Levels (PELs) - Table Z3	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Inert or Nuisance Dust: (d) Respirable fraction)		5						

US OSHA Permissible Exposure Levels (PELs) - Table Z3	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Inert or Nuisance Dust: (d) Total dust)	15			
US - Hawaii Air Contaminant Limits	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Particulates not otherwise regulated - Total dust)	10			
US - Hawaii Air Contaminant Limits	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Particulates not otherwise regulated - Respirable fraction)	5			
US - Oregon Permissible Exposure Limits (Z3)	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Inert or Nuisance Dust: (d) Respirable fraction)	5			*
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Particulates not otherwise regulated Respirable fraction)	5			
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Particulates not otherwise regulated (PNOR)(f)-Respirable fraction)	5			
US - Michigan Exposure Limits for Air Contaminants	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Particulates not otherwise regulated, Respirable dust)	5			
Canada - Northwest Territories Occupational Exposure Limits (English)	Nalpa-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (Nitrobenzene - Skin)	1	5	2	10

MATERIAL DATA

NALPHA-(2,4-DINITRO-5-FLUOROPHENYL)-L-ALANINAMIDE:

■ It is the goal of the ACGIH (and other Agencies) to recommend TLVs (or their equivalent) for all substances for which there is evidence of health effects at airborne concentrations encountered in the workplace.

At this time no TLV has been established, even though this material may produce adverse health effects (as evidenced in animal experiments or clinical experience). Airborne concentrations must be maintained as low as is practically possible and occupational exposure must be kept to a minimum.

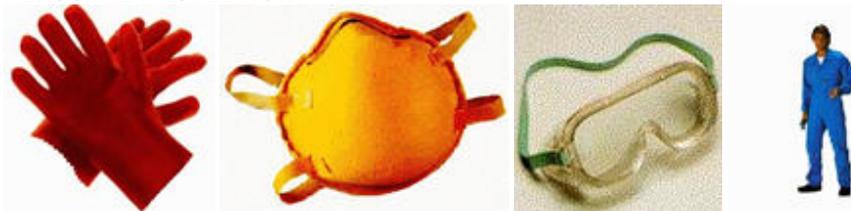
NOTE: The ACGIH occupational exposure standard for Particles Not Otherwise Specified (P.N.O.S) does NOT apply.

Sensory irritants are chemicals that produce temporary and undesirable side-effects on the eyes, nose or throat. Historically occupational exposure standards for these irritants have been based on observation of workers' responses to various airborne concentrations. Present day expectations require that nearly every individual should be protected against even minor sensory irritation and exposure standards are established using uncertainty factors or safety factors of 5 to 10 or more. On occasion animal no-observable-effect-levels (NOEL) are used to determine these limits where human results are unavailable. An additional approach, typically used by the TLV committee (USA) in determining respiratory standards for this group of chemicals, has been to assign ceiling values (TLV C) to rapidly acting irritants and to assign short-term exposure limits (TLV STELs) when the weight of evidence from irritation, bioaccumulation and other endpoints combine to warrant such a limit. In contrast the MAK Commission (Germany) uses a five-category system based on intensive odour, local irritation, and elimination half-life. However this system is being replaced to be consistent with the European Union (EU) Scientific Committee for Occupational Exposure Limits (SCOEL); this is more closely allied to that of the USA.

OSHA (USA) concluded that exposure to sensory irritants can:

- cause inflammation
- cause increased susceptibility to other irritants and infectious agents
- lead to permanent injury or dysfunction
- permit greater absorption of hazardous substances and
- acclimate the worker to the irritant warning properties of these substances thus increasing the risk of overexposure.

PERSONAL PROTECTION



Consult your EHS staff for recommendations

EYE

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses pose a special hazard; soft lenses may absorb irritants and all lenses concentrate them. DO NOT wear contact lenses.

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.
- Respirators may be necessary when engineering and administrative controls do not adequately prevent exposures.
- The decision to use respiratory protection should be based on professional judgment that takes into account toxicity information, exposure measurement data, and frequency and likelihood of the worker's exposure - ensure users are not subject to high thermal loads which may result in heat stress or distress due to personal protective equipment (powered, positive flow, full face apparatus may be an option).
- Published occupational exposure limits, where they exist, will assist in determining the adequacy of the selected respiratory . These may be government mandated or vendor recommended.
- Certified respirators will be useful for protecting workers from inhalation of particulates when properly selected and fit tested as part of a complete respiratory protection program.
- Use approved positive flow mask if significant quantities of dust becomes airborne.
- Try to avoid creating dust conditions.

RESPIRATOR

Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
10 x PEL	P1 Air-line*	-	PAPR-P1 -
50 x PEL	Air-line**	P2	PAPR-P2
100 x PEL	-	P3 Air-line*	-
100+ x PEL	-	Air-line**	PAPR-P3

* - Negative pressure demand ** - Continuous flow

Explanation of Respirator Codes:

Class 1 low to medium absorption capacity filters.

Class 2 medium absorption capacity filters.

Class 3 high absorption capacity filters.

PAPR Powered Air Purifying Respirator (positive pressure) cartridge.

Type A for use against certain organic gases and vapors.

Type AX for use against low boiling point organic compounds (less than 65°C).

Type B for use against certain inorganic gases and other acid gases and vapors.

Type E for use against sulfur dioxide and other acid gases and vapors.

Type K for use against ammonia and organic ammonia derivatives

Class P1 intended for use against mechanically generated particulates of sizes most commonly encountered in industry, e.g. asbestos, silica.

Class P2 intended for use against both mechanically and thermally generated particulates, e.g. metal fume.

Class P3 intended for use against all particulates containing highly toxic materials, e.g. beryllium.

The local concentration of material, quantity and conditions of use determine the type of personal protective equipment required.

Use appropriate NIOSH-certified respirator based on informed professional judgement. In conditions where no reasonable estimate of exposure can be made, assume the exposure is in a concentration IDLH and use NIOSH-certified full face pressure demand SCBA with a minimum service life of 30 minutes, or a combination full facepiece pressure demand SAR with auxiliary self-contained air supply. Respirators provided only for escape from IDLH atmospheres shall be NIOSH-certified for escape from the atmosphere in which they will be used.

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.
- If in spite of local exhaust an adverse concentration of the substance in air could occur, respiratory protection should be considered. Such protection might consist of:
 - (a): particle dust respirators, if necessary, combined with an absorption cartridge;
 - (b): filter respirators with absorption cartridge or canister of the right type;
 - (c): fresh-air hoods or masks
- Build-up of electrostatic charge on the dust particle, may be prevented by bonding and grounding.
- Powder handling equipment such as dust collectors, dryers and mills may require additional protection measures such as explosion venting.

Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to efficiently remove the contaminant.

Type of Contaminant:	Air Speed:
direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)	1-2.5 m/s (200-500 f/min.)
grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).	2.5-10 m/s (500-2000 f/min.)
Within each range the appropriate value depends on:	
Lower end of the range	Upper end of the range
1: Room air currents minimal or favorable to capture	1: Disturbing room air currents
2: Contaminants of low toxicity or of nuisance value only	2: Contaminants of high toxicity
3: Intermittent, low production.	3: High production, heavy use
4: Large hood or large air mass in motion	4: Small hood-local control only

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at

the extraction fan, for example, should be a minimum of 4-10 m/s (800-2000 f/min) for extraction of crusher dusts generated 2 meters distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Solid.

Does not mix with water.

State	Divided solid	Molecular Weight	272.19
Melting Range (°F)	440.6- 442.4	Viscosity	Not Applicable
Boiling Range (°F)	Not available	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	Not available	pH (1% solution)	Not applicable
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)	Not Applicable
Volatile Component (%vol)	Negligible	Evaporation Rate	Not applicable

APPEARANCE

Yellow powder; does not mix well with water. Soluble in acetone.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

-
- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerization will not occur.

STORAGE INCOMPATIBILITY

-
- Polynitro derivatives of mono- and poly- cyclic systems are often explosives liable to detonate on grinding or impact.
- The presence of two or more nitro groups (each with 2 oxygen atoms) on an aromatic nucleus often increase the reactivity of other substituents and the tendency towards explosive instability as oxygen balance is approached.
- 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.
- In view of the reports of previous violent or explosive reactions, heating of polynitroaryl (particularly di- and tri-nitroaryl) compounds with alkalis, ammonia, or O-ethylsulfuric acid salts, in autoclaves should be avoided.
- 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 alkalis, 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.
- 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.

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

- Many arylamines (aromatic amines such as aniline, N-ethylaniline, o-toluidine, xylydine etc. and their mixtures) are hypergolic (ignite spontaneously) with red fuming nitric acid. When the amines are dissolved in triethylamine, ignition occurs at -60 deg. C. or less.
- Various metal oxides and their salts may promote ignition of amine-red fuming nitric acid systems. Soluble materials such as copper(I) oxide, ammonium metavanadate are effective; insoluble materials such as copper(II) oxide, iron(II) oxide, potassium dichromate are also effective.
- Avoid oxidizing agents, acids, acid chlorides, acid anhydrides.
- Avoid strong bases.

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

Section 11 - TOXICOLOGICAL INFORMATION

Nalpha-(2,4-dinitro-5-fluorophenyl)-L-alaninamide

TOXICITY AND IRRITATION

- 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

Refer to data for ingredients, which follows:

NALPHA-(2,4-DINITRO-5-FLUOROPHENYL)-L-ALANINAMIDE:

■ Harmful to aquatic organisms.

■ Aromatic amines (arylamines), particularly primary aromatic amines, covalently and irreversibly bind to humic substances present in most natural waters.

All metabolites with moieties of: anilines, benzidines and toluidines are of environmental concern. Anilines and benzidines are both acutely toxic and toxic depending on the specific aquatic species (except algae). Toluidines represent a similar concern. It has been speculated that aqueous solutions of aromatic amines can be oxidised by organic radicals, but there are no actual data on reaction rates. Based on a study of reaction rate data for these compounds an estimate of the half-life of aromatic amines in water is approximately 100 days, assuming a peroxy radical concentration of 10⁻¹⁰ mole/L in sunlight, oxygenated water.

■ The nitrates are of environmental concern because of their high water solubility and consequent leaching, diffusion, and environmental mobility in soil and water. Nitrate can contaminate groundwater to unacceptable levels. Nitrite is formed from nitrate or ammonium ion by micro-organisms in soil, water, sewage and the alimentary tract. The concern with nitrate in the environment is related to its conversion to nitrite.

Methemoglobinemia is caused following exposure to high levels of nitrite and produces difficulties in oxygen transport in the blood. Thousands of cases involving poisoning of infants, particularly in rural areas, have been reported as a result of drinking nitrate rich well-water.

Other concerns deriving from exposure to environmental nitrates relate to the production of nitrosamines following the reaction of food nitrites and secondary amines. Other nitroso-compounds may result following reaction with nitrites and amides, ureas, carbamates and other nitrogenous compounds. Nitrosamines produce liver damage, hemorrhagic lung lesions, convulsions and coma in rats, and teratogenic effects in experimental animals.

The N-nitroso class of compounds include potent carcinogens and mutagens: induction of tumors by single doses of N-nitroso compounds testify to this.

■ DO NOT discharge into sewer or waterways.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
Nalpha-(2,4-dinitro-5-fluorophenyl)-L-alaninamide	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.
- Dispose of by: Burial in a licensed land-fill or Incineration in a licensed apparatus (after admixture with suitable combustible material)
- Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

Section 14 - TRANSPORTATION INFORMATION

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IATA, IMDG

Section 15 - REGULATORY INFORMATION

Nalpha-(2,4-dinitro-5-fluorophenyl)-L-alaninamide (CAS: 95713-52-3) is found on the following regulatory lists;

"Canada Environmental Quality Guidelines (EQGs) Water: Aquatic life","Canada Environmental Quality Guidelines (EQGs) Water: Community","US DOE Temporary Emergency Exposure Limits (TEELs)"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

- Ingestion may produce health damage*.
 - Cumulative effects may result following exposure*.
- * (limited evidence).

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- Classification of the mixture 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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