

1. Material Identification

Product Name : Nitrofen

Catalog Number : io-2733

CAS Number : 1836-75-5

Identified uses : Laboratory chemicals, manufacture of chemical compounds

Company : IonZ

>> R&D Use only

2. Hazards Identification

GHS Classification:

Flammable liquid (category 2)

Acute toxicity, oral (Category 3)

Acute toxicity, dermal (Category 3)

Acute toxicity, inhalation (Category 3)

Specific target organ toxicity, single exposure (Category 1)

Pictogram(s)



GHS Hazard Statements

>> H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H350 (100%): May cause cancer [Danger Carcinogenicity]

>> H360 (97.9%): May damage fertility or the unborn child [Danger Reproductive toxicity]

>> H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (97.9%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P264, P270, P273, P280, P301+P317, P318, P330, P391, P405, and P501

Health Hazards:

>> SYMPTOMS: Symptoms of exposure to this compound may include irritation of the skin and eyes.

>> ACUTE/CHRONIC HAZARDS: This compound is toxic by ingestion. It may cause irritation of the skin and eyes. When heated to decomposition it emits toxic fumes of nitrogen oxides and chlorine. (NTP, 1992)

>> Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

>> Combustible. Finely dispersed particles form explosive mixtures in air.

3. Composition/Information On Ingredients

Chemical name : Nitrofen
CAS Number : 1836-75-5
Molecular Formula : C₁₂H₇Cl₂NO₃
Molecular Weight : 284.0900 g/mol

4. First Aid Measures

First Aid:

- >> EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.
- >> SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.
- >> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.
- >> INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital.
- >> OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the possible long term health effects and potential recommendation for medical monitoring. Recommendations from the physician will depend upon the specific compound, its chemical, physical and toxicity properties, the exposure level, length of exposure, and the route of exposure. (NTP, 1992)

First Aid Measures

Inhalation First Aid

- >> Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Skin First Aid

- >> First rinse with plenty of water for at least 15 minutes, then remove contaminated clothes and rinse again. Refer for medical attention .

Eye First Aid

- >> First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion First Aid

- >> Rinse mouth. Rest. Refer for medical attention .

5. Fire Fighting Measures

- >> Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)
- >> Use water spray, powder, foam, carbon dioxide.

6. Accidental Release Measures

Isolation and Evacuation:

Isolation and evacuation measures to take when a large amount of this chemical is accidentally released in an emergency.

- >> Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]:
- >> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.
- >> SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.
- >> FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

- >> Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: P3 filter respirator for toxic particles.

7. Handling And Storage

Safe Storage:

- >> Separated from food and feedstuffs. Well closed.

Storage Conditions:

- >> PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemico-physical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

8. Exposure Control/ Personal Protection

Inhalation Risk:

- >> Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly on spraying or when dispersed, especially if powdered.

Effects of Short Term Exposure:

- >> The substance is irritating to the skin and respiratory tract. The substance may cause effects on the central nervous system.

Effects of Long Term Exposure:

- >> Repeated or prolonged contact with skin may cause dermatitis. The substance may have effects on the liver. This substance is possibly carcinogenic to humans. Animal tests show that this substance possibly causes malformations in human babies.

Fire Prevention

- >> NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust.

Exposure Prevention

- >> PREVENT DISPERSION OF DUST! AVOID ALL CONTACT! AVOID EXPOSURE OF (PREGNANT) WOMEN! IN ALL CASES CONSULT A DOCTOR!

Inhalation Prevention

>> Use local exhaust or breathing protection.

Skin Prevention

>> Protective gloves. Protective clothing.

Eye Prevention

>> Wear safety spectacles or eye protection in combination with breathing protection if powder.

Ingestion Prevention

>> Do not eat, drink, or smoke during work. Wash hands before eating.

9. Physical And Chemical Properties

Molecular Weight:

>> 284.09

Exact Mass:

>> 282.9802985

Physical Description:

>> Nitrofen appears as colorless crystals or black solid. Used as a pre- or post-emergence herbicide.

>> COLOURLESS-TO-BROWN CRYSTALLINE POWDER. TURNS DARK ON EXPOSURE TO LIGHT.

Color/Form:

>> Crystalline solid

Boiling Point:

>> 356 to 374 °F at 0.25 mmHg (NTP, 1992)

>> at 101.3kPa: 368 °C

Melting Point:

>> 158 to 160 °F (NTP, 1992)

>> 70–71 °C

Flash Point:

>> >200 °C c.c.

Solubility:

>> less than 1 mg/mL at 70 °F (NTP, 1992)

>> Solubility in water, g/100ml at 22 °C: 0.0001

Density:

>> 1.33 at 90 °C

>> 1.3 g/cm³

Vapor Pressure:

>> 8e-06 mmHg at 104 °F (NTP, 1992)

>> Vapor pressure, Pa at 40 °C: 0.001

LogP:

>> log Kow = 4.64

>> 3.4/5

Stability/Shelf Life:

>> DARKENS UNDER EXPOSURE TO LIGHT

Autoignition Temperature:

>> >400 °C

Decomposition:

>> When heated to decomp it emits very toxic fumes of /hydrogen chloride and nitrogen oxides./

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

EPA Provisional Peer-Reviewed Toxicity Values:

This section provides the EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs) and links of related assessment documents.

Chemical Substance

>> Nitrofen (technical grade)

Reference Dose (RfD), Chronic

>> 3×10^{-3} mg/kg-day

Reference Dose (RfD), Subchronic

>> 3×10^{-3} mg/kg-day

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> Likely to be carcinogenic to humans

Last Revision

>> 2012

RAIS Toxicity Values:

This section provides the Chemical toxicity information from the Risk Assessment Information System.

Inhalation Unit Risk (IUR) ($\mu\text{g}/\text{m}^3$)⁻¹

>> 2.3e-05

Inhalation Unit Risk Reference

>> CALEPA

Oral Chronic Reference Dose (RfDoc) (mg/kg-day)

>> 0.003

Oral Chronic Reference Dose Reference

>> PPRTV Current

Oral Subchronic Chronic Reference Dose (RfDos) (mg/kg-day)

>> 0.003

Oral Subchronic Chronic Reference Dose Reference

>> PPRTV Current

Oral Slope Factor (CSFo)(mg/kg-day)⁻¹

>> 0.038

Oral Slope Factor Reference

>> PPRTV Current

Evidence for Carcinogenicity:

Evidence that this chemical does or may cause cancer. The information here is collected from various sources by the Hazardous Substances Data Bank (HSDB).

>> No data are available in humans. Sufficient evidence of carcinogenicity in animals. OVERALL EVALUATION: Group 2B: The agent is possibly carcinogenic to humans.

Carcinogen Classification:

This section provides the International Agency for Research on Cancer (IARC) Carcinogenic Classification and related monograph links. In the IARC Carcinogenic classification, chemicals are categorized into four groups: Group 1 (carcinogenic to humans), Group 2A (probably carcinogenic to humans), Group 2B (possibly carcinogenic to humans), and Group 3 (not classifiable as to its carcinogenicity to humans).

IARC Carcinogenic Agent

>> Nitrofen (technical-grade)

IARC Carcinogenic Classes

>> Group 2B: Possibly carcinogenic to humans

IARC Monographs

>> Volume 30: (1983) Miscellaneous Pesticides

>> Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print)

Substance

>> Nitrofen

NTP Technical Report

>> TR-184: Bioassay of Nitrofen for Possible Carcinogenicity (CASRN 1836-75-5) (1979)

Peer Review Date

>> 10/25/78

Conclusion for Male Rat

>> No Evidence



Conclusion for Female Rat

>> No Evidence



Conclusion for Male Mice

>> Clear Evidence



Conclusion for Female Mice

>> Clear Evidence



Summary

>> Under the conditions of this bioassay, dietary administration of nitrofen was carcinogenic to B6C3F1 mice, causing hepatocellular carcinomas in both sexes. There was no evidence for carcinogenicity in Fischer 344 rats.

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its aerosol and by ingestion.

Inhalation Exposure

>> Abdominal pain. Cough. Diarrhoea. Dizziness. Headache. Laboured breathing. Sore throat. Vomiting.

Skin Exposure

>> Redness. Pain.

Eye Exposure

>> Redness. Pain.

Ingestion Exposure

>> See Inhalation.

Adverse Effects:

An adverse effect is an undesired harmful effect resulting from a medical treatment or other intervention.

>> Neurotoxin – Other CNS neurotoxin

- >> Occupational hepatotoxin – Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.
- >> Reproductive Toxin – A chemical that is toxic to the reproductive system, including defects in the progeny and injury to male or female reproductive function. Reproductive toxicity includes developmental effects. See Guidelines for Reproductive Toxicity Risk Assessment.
- >> IARC Carcinogen – Class 3: Chemicals are not classifiable by the International Agency for Research on Cancer.
- >> NTP Carcinogen – Reasonably anticipated to be a human carcinogen.

Toxicity Data:

- >> LCLo (cats) = 620 mg/m³/4h

Interactions:

- >> ... The aim of this study was to examine whether antenatal treatment with vitamin A can increase lung growth and reduce the incidence of CDH in a nitrofen-treated rat model. The animals were randomly assigned to four groups: control, vitamin A, nitrofen, and nitrofen/vitamin A (NIP/Vit A). The incidence of CDH /congenital diaphragmatic hernia/ in the NIP/Vit A group (54%) was markedly lower than that in the nitrofen-treated group (85%). Although lung weight was decreased in the nitrofen-treated and NIP/vitamin A groups, the fetal lung weight-to-body weight ratio was slightly increased in the NIP/vitamin A group, compared to the nitrofen-treated group. The mRNA levels of lung surfactant proteins were decreased in the NIP/vitamin A group. We conclude that antenatal treatment with vitamin A reduced the incidence of CDH without lung maturation in the nitrofen-induced rat model.

Antidote and Emergency Treatment:

- >> Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Aromatic hydrocarbons and related compounds/

Human Toxicity Excerpts:

- >> /HUMAN EXPOSURE STUDIES/ IN 48-HR SKIN PATCH TESTS ON WOMEN FROM AGRICULTURAL AREA (FRUIT ORCHARDS & RICE PADDIES) NITROFEN WAS AMONG THOSE PESTICIDES GIVING HIGHEST POS RESULTS.

Non-Human Toxicity Excerpts:

- >> /LABORATORY ANIMALS: Acute Exposure/ ... RATS /EXPOSED TO A MIXTURE OF/ 25% ACTIVE INGREDIENT /OF NITROFEN/ IN XYLENE AT 3-10 PARTS WATER, EXPOSURE TIME OF 1 HR, RESULTED IN NO SIGNS OF ACUTE OR SUBACUTE IRRITATION OF RESP TRACT NOR ANY PATHOLOGICAL CHANGES IN LIVER OR KIDNEY TISSUE.

Non-Human Toxicity Values:

- >> LD50 Rabbit dermal >5000 mg/kg bw

National Toxicology Program Studies:

Reports from the National Toxicology Program, an interagency program supported by three government agencies (NIH, FDA, and CDC) within the Department of Health and Human Services. This program plays a critical role in generating, interpreting, and sharing toxicological information about chemicals of public health concerns.

- >> A bioassay for the possible carcinogenicity of nitrofen was conducted using Fischer 344 rats and B6C3F1 mice. Nitrofen was administered in the feed, at either of two concentrations, to groups of 50 male and 50 female animals of each species. Twenty animals of each sex and species were placed on test as controls. The high and low dietary concentrations of nitrofen were 6000 and 3000 ppm for both species. The compound was administered to rats and mice for 78 weeks, followed by a period of no compound administration of 26 weeks for rats and 13 weeks for mice. There were no significant positive associations between the concentrations of nitrofen administered and mortality in rats or mice of either sex. Adequate numbers of animals in all groups survived sufficiently long to be at risk from late-developing tumors. Dose-related mean body weight depression, relative to controls, was observed for males and females of both species, indicating that the concentrations of nitrofen administered to the animals in this bio-assay may have approximated the maximum tolerated concentrations. None of the statistical tests for any site in rats of either sex indicated a significant positive association between compound administration and tumor incidence. There was a significant positive association between the concentrations of nitrofen administered and the incidences of hepatocellular carcinomas in mice of both sexes. Under the conditions of this bioassay, dietary administration of nitrofen was carcinogenic to B6C3F1 mice, causing hepatocellular carcinomas in both sexes. There was no evidence for carcinogenicity in Fischer 344 rats.

12. Ecological Information

ICSC Environmental Data:

- >> The substance is very toxic to aquatic organisms. Bioaccumulation of this chemical may occur along the food chain, for example in fish. The substance may cause long-term effects in the aquatic environment. Avoid release to the environment in circumstances different to normal use.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

- >> SEDIMENT: Sediment samples from Beijing Guanting Reservoir taken at seven locations in Sept and Nov 2003, and June and Aug 2004 contained nitrofen at 9.38 to 42.5 pg/g(1).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

- >> Nitrofen was detected in 3% of fish samples from nearly 400 sites throughout the US sampled 1986 to 1989, the highest concentration (18 ng/g) occurred in carp sampled from New Mormon Slough, Stockton, CA, the mean concentration was reported as 0.2 ng/g(1). Nitrofen was not detected in samples of fish, and shellfish from Japan(2).

Average Daily Intake:

The average amount of the compound taken into the body through eating, drinking, or breathing.

- >> In the adult Total Diet Study for fiscal year 1979 in which 20 market basket samples of 12 food groups were analyzed from all parts of the country, only one sample of leafy vegetables contained 6 ppb of nitrofen was identified which would result in an average daily intake of 0.0151 ug/day(1).

13. Disposal Considerations

Spillage Disposal

- >> Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: P3 filter respirator for toxic particles.

Disposal Methods

- >> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal and plant life; and conformance with environmental and public health regulations.
- >> Landfill: The dichloro aromatic constituent of the nitrofen molecule precludes rapid degradation in the environment. Burial away from water supplies is the preferred method of disposal. Large quantities should be incinerated. Recommendable method: Incineration.
- >> PRECAUTIONS FOR "CARCINOGENS": There is no universal method of disposal that has been proved satisfactory for all carcinogenic compounds & specific methods of chem destruction ... published have not been tested on all kinds of carcinogen-containing waste. ... summary of avail methods & recommendations ... /given/ must be treated as guide only. /Chemical Carcinogens/
- >> PRECAUTIONS FOR "CARCINOGENS": ... Incineration may be only feasible method for disposal of contaminated laboratory waste from biological expt. However, not all incinerators are suitable for this purpose. The most efficient type ... is probably the gas-fired type, in which a first-stage combustion with a less than stoichiometric air:fuel ratio is followed by a second stage with excess air. Some ... are designed to accept ... aqueous & organic-solvent solutions, otherwise it is necessary ... to absorb soln onto suitable combustible material, such as sawdust. Alternatively, chem destruction may be used, esp when small quantities ... are to be destroyed in laboratory. /Chemical Carcinogens/
- >> For more Disposal Methods (Complete) data for NITROFEN (7 total), please visit the HSDB record page.

14. Transport Information

DOT

Nitrofen

IATA

Nitrofen

15. Regulatory Information

Regulatory Information

California Safe Cosmetics Program (CSCP) Reportable Ingredient

- >> Hazard Traits – Bioaccumulation; Carcinogenicity; Environmental Persistence; Reproductive Toxicity
- >> Authoritative List – EC Annex VI CMRs – Cat. 1B; EC PBTs; IARC Carcinogens – 2B; NTP RoC – reasonable; Prop 65
- >> Report – regardless of intended function of ingredient in the product

New Zealand EPA Inventory of Chemical Status

- >> Nitrofen: HSNO Approval: HSR004593 Approved with controls

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

- >> Poisonous gases, including nitrogen oxides and chlorine, are produced in fire.

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