SAFETY DATA SHEET

Updated on 25/09/2024

1. Material Identification

Product Name : N-Nitrosodiphenylamine
Catalog Number : io-2754
CAS Number : 86-30-6
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)

Note

>> Pictograms displayed are for 98.1% (102 of 104) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for 1.9% (2 of 104) of reports.

Pictogram(s)

>> Warning

GHS Hazard Statements

>> H302 (60.6%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H315 (20.2%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H317 (38.5%): May cause an allergic skin reaction [Warning Sensitization, Skin]

>> H319 (22.1%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H351 (38.5%): Suspected of causing cancer [Warning Carcinogenicity]

>> H361 (37.5%): Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity]

>> H373 (38.5%): May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]

>> H410 (37.5%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

>> H411 (50%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P260, P261, P264, P264+P265, P270, P272, P273, P280, P301+P317, P302+P352, P305+P351+P338, P318, P319, P321, P330, P332+P317, P333+P317, P337+P317, P362+P364, P391, P405, and P501

Health Hazards:

>> ACUTE/CHRONIC HAZARDS: When heated to decomposition this compound emits toxic fumes of nitrogen oxides. (NTP, 1992)

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

>> Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : N-Nitrosodiphenylamine
CAS Number : 86-30-6
Molecular Formula : C12H10N2O
Molecular Weight : 198.2200 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. Refer for medical attention.

Skin First Aid

>> Remove contaminated clothes. Rinse and then wash skin with water and soap.

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. 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 foam, powder, 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.

>> Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting.

7. Handling And Storage

Safe Storage:

>> Separated from strong oxidants. Store in an area without drain or sewer access.

Storage Conditions:

>> Keep container tightly closed in a dry and well-ventilated place. Store under inert gas. Air sensitive.

8. Exposure Control/ Personal Protection

MAK (Maximale Arbeitsplatz Konzentration)

>> carcinogen category: 3

Inhalation Risk:

>> Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

Fire Prevention

>> NO open flames.

Inhalation Prevention

>> Use local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety goggles.

Ingestion Prevention

>> Do not eat, drink, or smoke during work.

9. Physical And Chemical Properties

Molecular Weight:

>> 198.22

Exact Mass:

>> 198.079312947

Physical Description:

>> N-nitrosodiphenylamine appears as yellow to brown or orange powder or flakes or a black solid. Insoluble in water and denser in water. Hence sinks in water. (NTP, 1992)

>> YELLOW FLAKES.

Color/Form:

>> Yellow plates from ligroin

Boiling Point:

>> 101 °C

Melting Point:

>> 151.7 °F (NTP, 1992)

>> 66.5 °C

Solubility:

>> less than 1 mg/mL at 66 °F (NTP, 1992)

>> Solubility in water: none

Density:

>> 1.23 (NTP, 1992) - Denser than water; will sink

>> 1.23 g/cm³

Vapor Pressure:

>> 0.00007 [mmHg]

LogP:

>> log Kow = 3.13

>> 2.57/3.13

Stability/Shelf Life:

>> Stable under recommended storage conditions.

Decomposition:

>> Hazardous decomposition products formed under fire conditions - Carbon oxides, nitrogen oxides (NOx).

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION AND USE: N-nitrosodiphenylamine (NDPHA) is a solid. NDPHA is an effective radical scavenger, and can be used to stabilize monomers, polymers and petroleum products. In rubber processing, its major use is believed to be as an anti-scorching agent, or vulcanization retarder, during rubber compounding. It is also used to make p-nitrosodiphenylamine. HUMAN STUDIES: NDPHA did not induce unscheduled DNA synthesis in human foreskin fibroblasts treated with up to 400 ug/mL. ANIMAL STUDIES: In an acute study of hepatotoxicity, mice given 350 mg/kg/day of NDPHA for 4 consecutive days preceding, or one dose 24 hours prior to, pentobarbital administration had effects characteristic of liver enzyme induction. In another study, rats and mice were fed diets containing up to 46000 mg/kg NDPHA for seven or 11 weeks. Female rats did not survive doses greater than 16000 mg/kg of diet; female mice survived higher doses. Male rats and male mice were not killed by the highest doses tested (10000 and 22000 mg/kg of diet, respectively). Rats were exposed to NDPHA by dietary feed at concentrations of 0, 250, 1000, 2000, 3000 or 4000 ppm for 5 days, 2, 4 and 13 weeks duration. There were no NDPHA exposure-related clinical signs of toxicity. NDPHA at a dose of 250 ug/mL did not induce DNA repair in Escherichia coli in the presence of metabolic activation. In several studies, doses of up to 2500 ug/plate NDPHA did not induce reversions in Salmonella typhimunum strains TA98, TA100, TA1535, TA1536, TA1537, TA 1538, G46, C3076 or 03052 in the presence of metabolic activation.

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

>> n-Nitrosodiphenylamine

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> See the IRIS entry for n-Nitrosodiphenylamine

Last Revision

>> 2007

USGS Health-Based Screening Levels for Evaluating Water-Quality:

This section provides the USGS Health-Based Screening Levels for Evaluating Water-Quality data.

Chemical

>> N-Nitrosodiphenylamine

Cancer HBSL [µg/L]

>> 6-600

Reference

>> Smith, C.D. and Nowell, L.H., 2024. Health-Based Screening Levels for evaluating water-quality data (3rd ed.). DOI:10.5066/F71C1TWP

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. Limited evidence of carcinogenicity in animals. OVERALL EVALUATION: Group 3: The agent is not classifiable as to its carcinogenicity 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

>> N-Nitrosodiphenylamine

IARC Carcinogenic Classes

>> Group 3: Not classifiable as to its carcinogenicity to humans

IARC Monographs

>> Volume 27: (1982) Some Aromatic Amines, Anthraquinones and Nitroso Compounds, and Inorganic Fluorides Used in Drinking-water and Dental Preparations

>> 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)

Exposure Routes:

>> The substance can be absorbed into the body by ingestion.

Target Organs:

Organs that are affected by exposure to this chemical. Information in this section reflects human data unless otherwise noted.

>> Body Weight

Cancer Sites:

The site in which cancer develops due to exposure to this compound. Cancers are casually referred to based on their primary sites (e.g., skin, lung, breasts, prostate, colon and rectum).

>> Urinary

Interactions:

>> The mutagenicity of the carcinogen N-nitrosodiphenylamine (NDPhA) to Salmonella typhimurium TA98 was demonstrated only when norharman, a comutagen, was added to the incubation mixture with S9 mix. N,N-Diphenylamine (DPhA), a denitrosated derivative of NDPhA, was also mutagenic to S. typhimurium TA98 when norharman was present. Twice as many revertants were induced by DPhA with norharman as by NDPhA with norharman. The comutagenic effect of norharman was also observed with N-nitroso-methylphenylamine (NMPhA), N-nitrosoethylphenylamine (NEPhA) and N-nitrosophenylbenzylamine (NPhBeA) and their denitrosated derivatives. NDPhA was converted metabolically to DPhA by S9 mix. Stoichiometric studies indicated that the mutagenicity of NDPhA in the presence of norharman was exerted through DPhA. The denitrosation eyzme activity of NDPhA was mainly recovered in the microsomal fraction, and the enzyme seemed to be a cytochrome P-450 monooxygenase system. Denitrosation reactions of NMPhA, NEPhA and NPhBeA were also demonstrated. The mutagenicities of these compounds with norharman are therefore suggested to be due to a mechanism similar to that of NDPhA with norharman.

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 the 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. /Organic bases/Amines and related compounds/

Human Toxicity Excerpts:

>> /GENOTOXICITY/ N-Nitrosodiphenylamine did not induce unscheduled DNA synthesis in human foreskin fibroblasts treated with up to 400 ug/mL ... .

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In an acute study of hepatotoxicity, mice given 350 mg/kg/day of N-nitrosodiphenylamine for 4 consecutive days preceding, or one dose 24 hours prior to, pentobarbital administration had effects characteristic of liver enzyme induction. These effects consisted of significantly decreased pentobarbital sleeping time and increased amounts of smooth endoplasmic reticulum among granules of glycogen in the liver cell. Electron microscopy also revealed blebs, hypertrophy, and pleomorphism of the mitochondria. A NOAEL of 350 mg/kg/day was identified for hepatic effects, since light microscopy examination did not reveal hepatic lesions.

Non-Human Toxicity Values:

>> LD50 Mouse ip 1000 mg/kg

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 of N-nitrosodiphenylamine for possible carcinogenicity was conducted by administration the test chemical in feed to F344 rats and B6C3F1 mice. Groups of 50 rats of each sex were administration N-nitrosodiphenylamine at one of two doses, either 1,000 or 4,000 ppm, for 100 wk. Matched controls consisted of 20 untreated rats of each sex. All surviving rats were killed at the end of administration of the test chemical. Groups of 50 male mice were administered N-ni trosodiphenylamine at one of two doses, either 10,000 or 20,000 ppm, for 101 weeks. Groups of 50 female mice were administered the test chemical at one of two doses, initially 5,000 or 10,000 ppm, for 38 weeks. Because of excessive depression in the amount of mean body weight gained in the dosed groups, the doses for the females were then reduced to 1,000 and 4,000 ppm, respectively, and administration at the lowered doses was

continued for 60 weeks. The time-weighted average doses for the female mice were either 2,315 or 5,741 ppm. Matched controls consisted of 20 untreated mice of each sex. All surviving mice were killed at the end of administration of the test chemical. Mean body weights of dosed rats and mice of each sex were lower than those of corresponding controls, and were dose related throughout the bioassay, except for those of female rats during the first part of the bioassay. Mortality was dose related in the female rats, but was not affected when the test chemical was administered to the male rats or the male or female mice. Survival at the end of the bioassay was 64% or greater in the dosed and control groups of rats and mice of each sex, and sufficient numbers of animals were at risk in all groups for the development of late-appearing tumors. Transitional-cell carcinomas of the urinary bladder occurred at incidences that were dose related (P less than 0.001) in both male and female rats, and in direct comparisons the incidences of these tumors in the high-dose groups of each sex were significantly higher (P less than or equal to 0.001) than those in the corresponding controls (males: controls 0/19, low-dose 0/46, high-dose 16/45; females: controls 0/18, low-dose 0/48, high-dose 40/49). The possible mechanism by which these tumors were induced, such as calculi formation in the bladder or nitrosation of amines present in feed to a carcinogenic nitrosoamine, is unknown. Fibromas of the integumentary system occurred in male rats at incidences that were dose related (P = 0.003), although in direct comparisons the incidences of these tumors in the individual dosed groups were not significantly higher than those in the control group (controls 1/20, or 5%; low-dose 1/50, or 2%; high-dose 10/50, or 20%). The incidence of fibromas of the integumentary system in historical-control male F344 rats at this laboratory is 6/285, or 2%. These results suggest an association of the fibromas in the male rats with the administration of the test chemical. No tumors occurred in the mice of either sex at incidences that were significantly higher in the dosed groups than in the corresponding control groups. The only changes related to compound administration were chronic inflammatory lesions in the urinary bladders of dosed mice. It is concluded that under the conditions of this bioassay, N-nitrosodiphenylamine was carcinogenic for both sexes of F344 rats, inducing transitional-cell carcinomas of the urinary bladder, but was not carcinogenic for B6C3F1 mice of either sex.

12. Ecological Information

Resident Soil (mg/kg)

>> 1.10e+02

Industrial Soil (mg/kg)

>> 4.70e+02

Resident Air (ug/m3)

>> 1.10e+00

Industrial Air (ug/m3)

>> 4.70e+00

Tapwater (ug/L)

>> 1.20e+01

MCL (ug/L)

>> 1.00e+03

Risk-based SSL (mg/kg)

>> 6.70e-02

Oral Slope Factor (mg/kg-day)-1

>> 4.90e-03

Inhalation Unit Risk (ug/m3)-1

>> 2.6e-06

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.1

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish. It is strongly advised not to let the chemical enter into the environment.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Sediment cores collected from five sampling stations of the western basin of Lake Ontario were found to contain no traces of N-nitrosodiphenylamine during analysis(1). N-Nitrosodiphenylamine was not detected (detection limit not reported) in sediment samples collected Feb 14-15, 2006 from 18 sampling sites located in Violet Marsh, LA after Hurricane Katrina(2).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> N-Nitrosodiphenylamine was monitored for, but not detected, in 9 species of fish collected from 14 locations on Lake Michigan and tributary streams during 1983(1).

13. Disposal Considerations

Spillage Disposal

>> Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting.

Disposal Methods

>> SRP: 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 air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

>> Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contaminated packaging: Dispose of as unused product.

>> Incineration: Pour or sift onto a thick layer of sand and soda ash mixture (90-10). Mix and shovel into a heavy paper box with much paper packing. Burn in an incinerator. Fire may be augmented by adding excelsior and scrap wood. Waste may be dissolved in flammable solvent (alcohols, etc) and sprayed into fire box of an incinerator with afterburner and scrubber.

>> (1) Nitrosamines may be reduced to the corresponding amine by using nickel-aluminum (Ni-Al) alloy in dilute base. The nitrosamines were completely degraded (99.9%) and only the amines (RR'NH) were found in the final reaction mixtures. No traces (generally <0.1%) of the corresponding, possibly carcinogenic, hydrazines (RR'NNH2) were found in the final reaction mixtures. (2) Nitrosamines may be oxidized by potassium permanganate in 3 M sulfuric acid ($KMnO_4$ in H_2SO_4). The nitrosamines were completely destroyed (>99.5%). The products of this reaction have not been determined. (3) Nitrosamines may be destroyed by using hydrogen bromide (HBr) in glacial acetic acid. The nitrosamines were completely destroyed (>99%) and the products were presumably the corresponding amines. All of these procedures were validated by an international collaborative study. /Nitrosamines/

>> For more Disposal Methods (Complete) data for N-Nitrosodiphenylamine (9 total), please visit the HSDB record page.

14. Transport Information

DOT

N-Nitrosodiphenylamine

Reportable Quantity of 100 lb or 45

IATA

N-Nitrosodiphenylamine

,

15. Regulatory Information

Clean Water Act Requirements:

The Clean Water Act (CWA) of 1972 establishes the basic structure for regulating discharges of pollutants into the waters of the United States and regulating quality standards for surface waters. Under CWA, the U.S. Environmental Protection Agency (EPA) developed the Toxic Pollutant List (40 CFR Part 401.15) and the Priority Pollutant List (40 CFR Part 423, Appendix A). These lists are to be used by EPA and States to develop the Effluent Guidelines regulations and ensure water quality criteria and standards.

>> Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations. /Nitrosamines/

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: Benzenamine, N-nitroso-N-phenyl-

REACH Registered Substance

>> Status: Active Update: 16-10-2018 https://echa.europa.eu/registration-dossier/-/registered-dossier/27089

New Zealand EPA Inventory of Chemical Status

>> Benzenamine, N-nitroso-N-phenyl-: Does not have an individual approval but may be used as a component in a product covered by a group standard. It is not approved for use as a chemical in its own right.

16. Other Information

Toxic Combustion Products:

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

>> Special hazards arising from the substance or mixture: Carbon oxides, Nitrogen oxides (NOx).

Other Safety Information

Chemical Assessment

>> IMAP assessments - Benzenamine, N-nitroso-N-phenyl-: Human health tier II assessment

"The information provided is believed to be accurate but is not comprehensive and should be used as a reference. It reflects our current knowledge and is intended for safety guidance related to the product. This document does not constitute a warranty of the product's properties. Ionz is not responsible for any damages resulting from handling or contact with the product incorrectly."