ionz

SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : n-Dioctylphthalate
Catalog Number : io-2282
CAS Number : 117-84-0
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

>> This chemical does not meet GHS hazard criteria for 57.1% (36 of 63) of all reports. Pictograms displayed are for 42.9% (27 of 63) of reports that indicate hazard statements.

Pictogram(s)

>> Warning

GHS Hazard Statements

>> H361 (41.3%): Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity]

Precautionary Statement Codes

>> P203, P280, P318, P405, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA Fire Rating

>> 1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.

NFPA Instability Rating

>> 0 - Materials that in themselves are normally stable, even under fire conditions.

Health Hazards:

>> Produces no ill effects at normal temperatures but may give off irritating vapor at high temperature. (USCG, 1999)

>> Special Hazards of Combustion Products: None (USCG, 1999)

3. Composition/Information On Ingredients

Chemical name : n-Dioctylphthalate
CAS Number : 117-84-0
Molecular Formula : C24H38O4
Molecular Weight : 390.6000 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. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. 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. (NTP, 1992)

5. Fire Fighting Measures

>> Carbon oxides

>> Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]:

>> CAUTION: Fire involving Safety devices (UN3268) and Fire suppressant dispersing devices (UN3559) may have a delayed activation and a risk of hazardous projectiles. Extinguish the fire at a safe distance.

>> SMALL FIRE: Dry chemical, CO2, water spray or regular foam.

>> LARGE FIRE: Water spray, fog or regular foam. Do not scatter spilled material with high-pressure water streams. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

>> FIRE INVOLVING TANKS: Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

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)

7. Handling And Storage

Storage Conditions:

>> Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

8. Exposure Control/ Personal Protection

>> 8 hr Time Weighted Avg (TWA): 5 mg/cu m.

9. Physical And Chemical Properties

Molecular Weight:

>> 390.6

Exact Mass:

>> 390.27700969

Physical Description:

>> Di-n-octyl phthalate appears as a clear liquid with a mild odor. Slightly less dense than water and insoluble in water. Hence floats on water. Flash point 430 °F. The primary hazard is the threat to the environment. Immediate steps should be taken to limit its spread to the environment. As a liquid, can easily penetrate the soil and contaminate groundwater and nearby streams. Eye contact may produce severe irritation and direct skin contact may produce mild irritation. Used in the manufacture of a variety of plastics and coating products.

Color/Form:

>> Clear, oily liquid

Boiling Point:

>> 428 °F at 760 mmHg (NTP, 1992)

Melting Point:

>> -13 °F (NTP, 1992)

Flash Point:

>> 219 °F (NTP, 1992)

Solubility:

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

Density:

>> 0.98 at 77 °F (USCG, 1999) - Less dense than water; will float

Vapor Pressure:

>> less than 0.2 mmHg at 302 °F (NTP, 1992)

LogP:

>> log Kow = 8.10

Stability/Shelf Life:

>> Stable under recommended storage conditions.

Autoignition Temperature:

>> 735 °F (390 °C)

Decomposition:

>> When heated to decomp it emits acrid smoke and irritating fumes.

Viscosity:

>> 39 mPa.s at 20 °C

Refractive Index:

>> Index of refraction = 1.485 at 20 °C/D

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION AND USE: Di-n-octylphthalate (DNOP) is a clear, oily liquid. It is used as a plasticizer; DNOP can represent 5-60% of the total weight of the plastics and resins. It is found in cosmetics and colorants. DNOP also serves as a carrier for catalysts or initiators and as a substitute for electrical capacitor fluid. HUMAN EXPOSURE AND TOXICITY: In 173 subjects with suspected dermatoses to plastic or glue allergens, two subjects (1.2% of the group) experienced irritation after patch testing with 2.0% DNOP. None of the patients had allergic reactions. There is a case study of a worker with continuous exposure to DNOP during the manufacture of imitation leather, who developed an asthmatic reaction to the substance. Women with endometriosis showed significantly higher concentrations of DNOP in their blood in a study of 49 infertile women with endometriosis (study group), and 38 age-matched women without endometriosis (control group I) but with infertility related to tubal defects, fibroids, polycystic ovaries, idiopathic infertility and pelvic inflammatory diseases diagnosed by laparoscopy and a further group of 21 age-matched women (control group II). An increase in toxic polyneuritis has been reported in workers exposed primarily to dibutyl phthalates. Lesser levels of exposure to dioctyl, diisooctyl, benzylbutyl phthalates, and tricresyl phosphate were also noted. ANIMAL STUDIES: DNOP was reported to be a slight skin irritant when applied to the depilated skin of guinea pigs. However, DNOP was not a skin sensitizer in guinea pigs. Ocular administration of DNOP resulted in slight conjunctival irritation and no corneal damage. The results of several acute- and intermediate-duration oral studies in rodents indicate that the potential of DNOP to cause adverse reproductive and developmental effects is low. Unlike other phthalate esters such as DEHP, DNOP does not appear to affect testicular function or morphology. Observed hepatic effects in intermediate duration studies consisted of a statistically significant increase in hepatic ethoxyresorufin-O-deethylase activity and histological changes in hepatic architecture. Thyroid toxicity was also noted at this concentration. Rats treated with 100, 300, or 600 mg/kg DNOP by ip injection for up to 90 day were evaluated for immunological responses. The high dose resulted in early loss of distinction between the cortex and medulla of the thyroid, reduced numbers of follicles in the lymph nodes, and loss of morphology in the adrenal glands. However, there was no effect on immune response. Results of studies in Salmonella typhimurium strains TA98, TA100, TA1535, and TA1537 (with and without S-9 metabolic activation systems) indicated that DNOP is not mutagenic. ECOTOXICITY STUDIES: The toxicity of DNOP was assessed by measuring the effect of exposure to these compounds on the fecundity of Daphnia magna and on the hatching and survival of the early life stages of the fathead minnow Pimephales promelas. For Daphnia magna, exposure to 1.0 mg/L DNOP caused a significant reduction in reproduction. Exposure to DNOP did not affect survival of either early embryos or larvae of the fathead minnow at doses up to 10 mg/L (the highest dose tested). Hatching of the embryos was significantly decreased at 10 mg/L, but not at 3.2 mg/L DNOP.

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

>> di-N-Octyl Phthalate

Reference Dose (RfD), Chronic

>> 1 x 10^-2 mg/kg-day

Reference Dose (RfD), Subchronic

>> 1 x 10^-1 mg/kg-day

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> Inadequate information to assess carcinogenic potential

Last Revision

>> 2012

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

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

Chemical

>> Di-n-octyl phthalate

Noncancer HBSL (Health-Based Screening Level)[µg/L]

>> 60

Benchmark Remarks

>> Based on PPRTV

Reference

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

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).

>> No indication of carcinogenicity to humans (not listed by IARC).

Health Effects:

>> Phthalate esters are endocrine disruptors. Animal studies have shown that they disrupt reproductive development and can cause a number of malformations in affected young, such as reduced anogenital distance (AGD), cryptorchidism, hypospadias, and reduced fertility. The combination of effects associated with phthalates is called 'phthalate syndrome'. (A2883)

Exposure Routes:

>> Oral (L1903) ; inhalation (L1903) ; dermal (L1903)

>> Phthalate esters are endocrine disruptors and can cause a number of developmental malformations termed 'phthalate syndrome'. (A2883)

Target Organs:

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

>> Hepatic (Liver)

Adverse Effects:

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

>> 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.

Toxicity Data:

>> LD50: 13000 mg/kg (Oral, Mouse) (L1901) LD50: 73 500 mg/kg (Dermal, Guinea pig) (T29)

Interactions:

>> Male rats, initiated with a single intraperitoneal dose of the carcinogen diethylnitrosamine and then partially hepatectomized, did not experience any liver weight gain after 10 weeks of dietary exposure to 500 mg/kg/day of di-n-octylphthalate ... When exposure was extended to 26 weeks, small increases in absolute liver weight that were not significant ($p < 0.05$) were observed at di-n-octylphthalate doses of 250 mg/kg/day (2% increase) and 500 mg/kg/day (8% increase). However, when combined with diminished body weight gains, relative liver weight gains were increased by 5-16% when compared with control values.

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. /Esters and related compounds/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ In 173 subjects with suspected dermatoses to plastic or glue allergens, two subjects (1.2% of the group) experienced irritation after patch testing with 2.0% dioctyl phthalate. None of the patients had allergic reactions.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Some small, but statistically significant ($p < 0.05$), changes in testicular mitochondrial respiratory functions were observed in 35-day-old male rats 6 hours after they had received a single oral dose of 2,000 mg/kg di-n-octylphthalate by gavage ... . Oxygen consumption of mitochondrial preparations from the testis during state 3 respiration (succinate respiration in the presence of adenosine diphosphate (ADP); phosphorylation) was reduced by 20% when compared with untreated control values, and the respiratory control ratio of state 3 to state 4 respiration ("resting" succinate respiration in the absence of ADP), which is a measure of respiration dependency on ADP, was also slightly reduced by 8%. Pyruvate and lactate concentrations were not changed, nor was phosphorylative activity (the state 3 ratio of ADP to oxygen consumption). These effects were generally less extensive than those induced by di(2-ethylhexyl)phthalate treatment.

Non-Human Toxicity Values:

>> LD50 Rat ip 50.0 mL/kg /49,000 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.

>> Di-N-octylphthalate (DOP) was tested using the RACB protocol in Swiss CD-1 mice as part of a structure-activity evaluation of a variety of phthalates. Body weights, food & water consumptions, & clinical signs in a dose-range-finding study were used to set doses for the main study of 0.0, 1.25%, 2.5%, & 5% in feed. Feed consumption was unchanged by DOP addition. Based on measured consumption, these concns of DOP produced calculated consumption estimates of nearly equal to 1.8, 3.6, & 7.5 g DOP/kg bw/day. Three controls & two middle dose mice died during the continuous breeding phase. Both treated & contol mice gained an average of 12-14% of their original body weight. There was no effect of DOP exposure on the number of litters/pair, the mean number of live pups/litter (control value: 11.5 +/- 0.4 pups), proportion born alive, live pup weight adjusted for litter size (control: 1.60 +/- 0.01 gr) or days to deliver each litter. In the absence of any demonstrable reproductive toxicity, a Task 3 crossover mating was not performed, & the fertility of the second generation was evaluated for the controls & high dose groups. In the F1 mice, growth & viability were unaffected by DOP consumption. Reproduction was also unaffected: the same proportion of treated & control mice mated, & bore live litters. The size & viability of these litters was also unaffected by DOP (11.5 pups/litter, controls), as was adjusted pup weight (1.50 +/- 0.03 gr). The F1 adults were killed & necropsied after the F2 litters were delivered & evaluated. In F1 females, body weight was unaffected by 5% DOP exposure, but when adjusted for body weight, both liver weight & kidney weight was increased by 22% & 10%, respectively. Treated male terminal body weight was also unchanged by DOP, while adjusted liver weight was increased by 28%, & seminal vesicle weight was decreased by 12%. Epididymal sperm concn & motility were unchanged by DOP exposure at 5%; the proportion of morphologically abnormal forms was reduced in the treated mice, from a control value of 5% abnormal to 3.5% abnormal in the DOP-exposed males. Estrous cycle length & stage distribution (the proportion of time spent in each estrous stage) was unchanged by DOP exposure. The single finding of a slight reduction in F1 seminal vesicle weight is interesting in light of current concerns about second-generational reproductive toxicity, but needs confirmation. Overall, these data show that, at doses that induced significant hepatomegaly, di-n-octyl-phthalate was without any adverse reproductive effect in Swiss mice.

TSCA Test Submissions:

Under the Toxic Substances Control Act (TSCA), EPA has broad authority to issue regulations designed to require manufacturers (including importers) or processors to test chemical substances and mixtures for health and environmental effects. This section provides information on test reports submitted for this chemical under TSCA.

>> The mutagenicity of dioctyl phthalate was evaluated in Salmonella tester strains TA98, TA100, TA1535 and TA1537 (Ames Test), both in the presence and absence of added metabolic activation by Aroclor-induced rat liver S9 fraction. Dioctyl phthalate, diluted in DMSO, was tested at concentrations up to 3,200ug/plate using the plate incorporation technique. Dioctyl phthalate did not cause a positive response in any tester strain with or without metabolic activation.

12. Ecological Information

Resident Soil (mg/kg)

>> 6.30e+02

Industrial Soil (mg/kg)

>> 8.20e+03

Tapwater (ug/L)

>> 2.00e+02

MCL (ug/L)

>> 6.00e+00

Risk-based SSL (mg/kg)

>> 5.70e+01

Chronic Oral Reference Dose (mg/kg-day)

>> 1.00e-02

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.1

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Di-n-octyl phthalate was detected in an unspecified US river below a specialty chemical company at concentrations ranging from 1.5 to 25 ppm(1). Di-n-octyl phthalate was also detected at 2 sites in Morgan Creek, a tributary of Chester River which flows into Chesapeake Bay, below a plasticizer manufacturing plant at concentrations of 62 ppb and <5 ppb(2). Di-n-octyl phthalate was detected in sediment samples from the mouth of the Inner Harbor Navigation Canal at Lake Pontchartrain, LA in samples collected May to June 1980 at a concentration of 56 ng/g dry weight(3). Dioctyl phthalate, isomer unspecified, was detected in 10% of 31 sediment samples collected from the Detroit River in 1982 at mean concentrations ranging from 0.09 to 0.26 mg/kg(4). Di-n-octyl phthalate was found in 13.3% of 488 sites sampled from 19 major US river basins from Aug 1992 to Sept 1995 with a maximum concentration of 1100 ug/kg dry weight(5). Di-n-octyl phthalate was found in 28 of 40 sediment samples taken near 4 combined sewer overflow areas in the lower Passaic River in NJ(6).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Two of three seaperch (Embiotoea lateralis) taken from False Creek, Vancouver, Canada contained approximately 1 ppb of di-n-octyl phthalate(1).

Average Daily Intake:

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

>> The estimated mean human exposure to di-n-octyl phthalate via drinking water in Toronto, Canada is 0.0728 mg/year(1).

13. Disposal Considerations

Disposal Methods

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U107, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> The following wastewater treatment technologies have been investigated for di-n-octyl phthalate: Biological treatment, solvent extraction.

>> A good candidate for liquid injection incineration at a temperature range of 650 to 1,600 °C and a residence time of 0.1 to 2 seconds. A good candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids. A good candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids.

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

14. Transport Information

DOT

n-Dioctylphthalate

Reportable Quantity of 5000 lb or 2270 kg

IATA

n-Dioctylphthalate

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15. Regulatory Information

TSCA Requirements:

This section provides information on requirements concerning this chemical under the Toxic Substances Control Act (TSCA) of 1976. TSCA provides EPA with authority to require reporting, record-keeping and testing requirements, and restrictions relating to chemical substances and/or mixtures. Certain substances are generally excluded from TSCA, including, among others, food, drugs, cosmetics and pesticides.

>> Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. 1,2-Benzenedicarboxylic acid, dioctyl ester is included on this list. Effective date 10/04/82; Sunset date 10/04/92.

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: 1,2-Benzenedicarboxylic acid, dioctyl ester

>> Specific Information Requirement: Obligations to provide information apply. You must tell us within 28 days if the circumstances of your importation or manufacture (introduction) are different to those in our assessment.

REACH Restricted Substance

>> Restricted substance: Di-n-octyl phthalate (DNOP)

>> EC: 204-214-7

New Zealand EPA Inventory of Chemical Status

>> 1,2-Benzenedicarboxylic acid, dioctyl ester: Does not have an individual approval but may be used under an appropriate group standard

16. Other Information

Other Safety Information

Chemical Assessment

>> IMAP assessments - Phthalate esters: Environment tier II assessment

>> PEC / SN / Other assessments - Diisodecyl phthalate (DIDP) & Di-n-octyl phthalate (DnOP): Health

>> IMAP assessments - 1,2-Benzenedicarboxylic acid, dioctyl ester: Human health tier I 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."