

Chemical Safety Data Sheet MSDS / SDS

N-Isopropylaniline

Revision Date:2024-12-21 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : N-Isopropylaniline
CBnumber : CB2410290
CAS : 768-52-5
EINECS Number : 212-196-7
Synonyms : N-isopropylaniline, Benzenamine, N-(1-methylethyl)-

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral
Skin irritation, Category 2
Eye irritation, Category 2
Acute toxicity - Category 2, Inhalation
Specific target organ toxicity – single exposure, Category 3

Label elements**Pictogram(s)**

□

Signal word : Danger

Hazard statement(s)

H227 Combustible liquid
H302 Harmful if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation

H330 Fatal if inhaled

H331 Toxic if inhaled

H335 May cause respiratory irritation

Precautionary statement(s)

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P284 Wear respiratory protection.

P310 Immediately call a POISON CENTER or doctor/physician.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P405 Store locked up.

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P320 Specific treatment is urgent (see ... on this label).

P319 Get medical help if you feel unwell.

Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|---|
| Product name | : N-Isopropylaniline |
| Synonyms | : N-isopropylaniline, Benzenamine, N-(1-methylethyl)- |
| CAS | : 768-52-5 |
| EC number | : 212-196-7 |
| MF | : C9H13N |
| MW | : 135.21 |

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

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

Following ingestion

Rinse mouth. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin; headache, lassitude (weakness, exhaustion), dizziness; cyanosis; ataxia; dyspnea (breathing difficulty) on effort; tachycardia; methemoglobinemia Target Organs: Eyes, skin, respiratory system, blood, cardiovascular system, liver, kidneys (NIOSH, 2016)

Indication of any immediate medical attention and special treatment needed

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Aniline and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Fires involving this compound should be controlled with a dry chemical, carbon dioxide or halon extinguisher. (NTP, 1992)

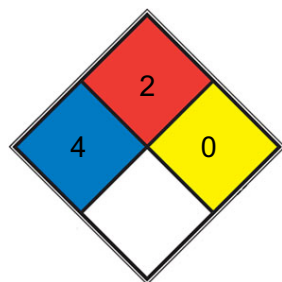
Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

Use powder, foam, carbon dioxide.

NFPA 704



| | | |
|---------------------------------|---|--|
| <input type="checkbox"/> HEALTH | 4 | Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, hydrofluoric acid) |
| <input type="checkbox"/> FIRE | 2 | Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur) |
| <input type="checkbox"/> REACT | 0 | Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N₂) |
| <input type="checkbox"/> SPEC. | | |
| <input type="checkbox"/> HAZ. | | |

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: complete protective clothing including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Above 82°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs. Cool. Keep in a well-ventilated room.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 2 ppm as TWA; (skin); BEI issued

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|---|
| Physical state | Liquid |
| Colour | Yellowish liquid |
| Odour | Sweet, aromatic odor. |
| Melting point/freezing point | -95°C(lit.) |
| Boiling point or initial boiling point and boiling range | 213°C(lit.) |
| Flammability | Class IIIB Combustible Liquid: Fl.P. at or above 200°F. |
| Lower and upper explosion limit/flammability limit | no data available |
| Flash point | 88°C(lit.) |
| Auto-ignition temperature | no data available |
| Decomposition temperature | no data available |
| pH | no data available |

| | |
|---------------------------------------|--|
| Kinematic viscosity | no data available |
| Solubility | less than 0.1 mg/mL at 70° F (NTP, 1992) |
| Partition coefficient n-octanol/water | no data available |
| Vapour pressure | 0.03 mm Hg at 77° F (NIOSH, 2016) |
| Density and/or relative density | 0.94 |
| Relative vapour density | 0.94 |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

N-ISOPROPYLANILINE neutralizes acids in exothermic reactions to form salts plus water. May be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen may be generated in combination with strong reducing agents, such as hydrides.

Conditions to avoid

no data available

Incompatible materials

STABILITY: This compound should be stable under normal laboratory conditions. (NTP, 1992)

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of nitroxides.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 560 mg/kg
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is mildly irritating to the eyes and skin. The substance may cause effects on the blood. This may result in the formation of methaemoglobin. The effects may be delayed. Medical observation is indicated. See Notes.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. The substance may have effects on the blood. This may result in the formation of methaemoglobin.

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

An estimated BCF of 18 was calculated for N-isopropylaniline(SRC), using an estimated log Kow of 2.53(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low.

Mobility in soil

The Koc of N-isopropylaniline is estimated as 566(SRC), using an estimated log Kow of 2.53(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that N-isopropylaniline is expected to have low mobility in soil. A pKa value of 5.3(4) suggests that N-isopropylaniline will partially exist in the protonated form in moist soils and the protonated form of N-isopropylaniline is expected to bind strongly to soil surfaces(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN3362 (For reference only, please check.)

IMDG: UN3362 (For reference only, please check.)

IATA: UN3362 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CHLOROSILANES, TOXIC, CORROSIVE, FLAMMABLE, N.O.S. (For reference only, please check.)

IMDG: CHLOROSILANES, TOXIC, CORROSIVE, FLAMMABLE, N.O.S. (For reference only, please check.)

IATA: CHLOROSILANES, TOXIC, CORROSIVE, FLAMMABLE, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.