

According to the UN GHS revision 8

Creation Date: May 15, 2024

Revision Date: May 15, 2024

1. IDENTIFICATION

1.1 GHS Product identifier

Product name: 4-Nitrobenzoic acid

Catalog Number: T20882

CAS Number: 62-23-7

1.2 Other means of identification

Other names: -

1.3 Recommended use of the chemical and restrictions on use

Identified uses:

1.4 Supplier's details

Company: Targetmol Chemicals Inc.

Uses advised against: 36 Washington Street, Wellesley Hills, Massachusetts 02481 USA

Tel/Fax: (781) 999-4286

1.5 Emergency phone number

Emergency phone number: 781-999-4286

Service hours: Monday to Friday, 9am-5pm (Standard timezone: UTC/GMT -5hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

Acute toxicity - Category 4, Oral

Eye irritation, Category 2

2.2 GHS label elements, including precautionary statements

Pictogram(s):



Signal word: Warning

Hazard statement(s):
H302 Harmful if swallowed
H319 Causes serious eye irritation

Precautionary statement(s):

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/...

Response:
P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Storage: none

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.

2.3 Other hazards which do not result in classification

no data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
4-Nitrobenzoic acid	-	62-23-7	200-526-2

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

no data available

If inhaled

Fresh air, rest.

Following skin contact

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

Following eye contact

Rinse with plenty of water (remove contact lenses if easily possible).

Following ingestion

Rinse mouth. Refer for medical attention .

4.2 Most important symptoms/effects, acute and delayed

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 if 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. Poisons A and B

4.3 Indication of immediate medical attention and special treatment needed, if necessary

SYMPTOMS: Symptoms of exposure to this compound include irritation of the skin, eyes, mucous membranes and upper respiratory tract. ACUTE/CHRONIC HAZARDS: This compound may be harmful by inhalation, ingestion or skin absorption. It is an irritant of the skin, eyes, mucous membranes and upper respiratory tract. When heated to decomposition it emits toxic fumes of carbon monoxide, carbon dioxide and nitrogen oxides. (NTP, 1992)

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

5.2 Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

5.3 Special protective actions for fire-fighters

Use foam, dry powder, carbon dioxide.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers.

6.2 Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers.

6.3 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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

NO open flames. 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.

7.2 Conditions for safe storage, including any incompatibilities

Separated from strong oxidants, bases and strong reducing agents.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Occupational Exposure limit values

MAK: (inhalable fraction): 4 mg/m³; peak limitation category: I(2); carcinogen category: 3B; pregnancy risk group: C

Biological limit values

no data available

8.2 Appropriate engineering controls

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

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust.

Thermal hazards

no data available

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Solid. Crystalline.
Color	Colorless, Yellow-white.
Odour	no data available
Melting point/ freezing point	Ca. 238 °C.
Boilingpoint or initial boiling point and boiling range	96°C/10mmHg(lit.)
Flammability	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	237°C

Auto-ignition temperature	300°C
Decomposition temperature	350°C
pH	Ca. 2.8.
Kinematic viscosity	no data available
Solubility	DMSO: Soluble,
N-octanol-water partition coefficient	log Pow = Ca. 1.89. Remarks:The temperature and pH is unknown.
Vapour pressure	Ca. 0 mm Hg. Temperature:Ca. 25 °C.
Density and/ or relative density	Ca. 1.6.
Relative vapour density	no data available
Particle characteristics	no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

Reacts with bases, reducing agents and strong oxidants strong oxidants. Decomposes on heating and on burning. This produces toxic fumes including nitrogen oxides nitrogen oxides.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

CombustibleDust explosion possible if in powder or granular form, mixed with air. If dry, it can be charged electrostatically by swirling, pneumatic transport, pouring, etc.P-NITROBENZOIC ACID is incompatible with strong oxidizers. It is also incompatible with strong bases (potassium hydroxide). It may react with cyanides. (NTP, 1992)

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Mixtures of the acid with potassium hydroxide (1:2 mol) readily deflagrated, .

10.6 Hazardous decomposition products

When heat to decomposition it emits toxic fumes of /nitrogen oxides/.

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral: no data available
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 irritating to the eyes, respiratory tract and skin.

STOT-repeated exposure

Animal tests show that this substance possibly causes toxicity to human reproduction or development.

Aspiration hazard

A nuisance-causing concentration of airborne particles can be reached quickly when dispersed, especially if powdered.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish: LC50 Brachydanio rerio (Zebrafish) >500 mg/L/48-hr; static bioassay (OECD guideline 203)

Toxicity to daphnia and other aquatic invertebrates: LC50 - Daphnia magna - ca. 1 295.053 mg/L - 48 h.

Toxicity to algae: EC5 - 537.796 mg/L - 96 h.

Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: Decomposition of nitrobenzoic acid took greater than 64 days by a soil microflora inoculum in mineral salts medium(1). After 180 minutes, little oxygen consumption by phenol adapted biological cultures occurred with 4-nitrobenzoic acid(2). The amounts of oxygen consumed after the 180 minute test time are 55 uL (endogenous), 64 uL (cells plus 100 mg/L 3-nitrobenzoic acid), and 346 uL (cells plus phenol - after 90 minutes) which results in a ratio of only 1.2 endogenous to 4-nitrobenzoic acid oxygen consumption(2). In a 2 week Japanese MITI test using 100 mg/L 4-nitrobenzoic acid and 30 mg/L sludge, 4-nitrobenzoic had a theoretical BOD of 62%(3). 4-Nitrobenzene reached 50.2% of its BOD in river water collected from Songhua River, China after 5 days. The river water samples contained about 8.0 mg/L dissolved oxygen, 800-3000/mL bacteria counts, pH 6.8-7.0, and temperatures of 15-20 deg C(4).

12.3 Bioaccumulative potential

An estimated BCF of 3.2 was calculated for 4-nitrobenzoic acid(SRC), using a log Kow of 1.89(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(SRC).

12.4 Mobility in soil

The Koc of 4-nitrobenzoic acid is estimated as 250(SRC), using a log Kow of 1.89(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 4-nitrobenzoic acid is expected to have moderate mobility in soil. The pKa of 4-nitrobenzoic acid is 3.44(4), indicating that this compound will exist almost entirely in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

12.5 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 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.

14. TRANSPORT INFORMATION

14.1 UN Number

no data available

14.2 UN Proper Shipping Name

no data available

14.3 Transport hazard class(es)

no data available

14.4 Packing group, if applicable

no data available

14.5 Environmental hazards

no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15. REGULATORY INFORMATION

15.1 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)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

16. OTHER INFORMATION

Information on revision

Creation Date May 15, 2024

Revision Date May 15, 2024

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>

A DRUG SCREENING EXPERT

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

no data available

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.

All products are for Research Use Only · Not For Human or Veterinary or Therapeutic Use