

SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.2
Creation Date: July 15, 2019
Revision Date: August 08, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name Pentachloronitrobenzene

1.2 Other means of identification

Product number CCPD100731

Other names Brassicol; PCNB; Batrilex

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.

Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.

Address 3/F, Building B, No. 179 BASIGO, Guangpu Rd East, Huangpu Dist, Guangzhou

Telephone +86-20-81960175

1.5 Emergency phone number

Emergency phone number +86-20-81960175

Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Skin sensitization, Category 1

Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning

Hazard statement(s) H317 May cause an allergic skin reaction

H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P273 Avoid release to the environment.

Response

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

P333+P317 If skin irritation or rash occurs: Get medical help.

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

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

P391 Collect spillage.

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

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Pentachloronitrobenzene	Quintozene	82-68-8	201-435-0	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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. Refer for medical attention.

4.2 Most important symptoms/effects, acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include irritation of the skin and eyes. Skin contact may result in erythema, itching, edema and formation of small vesicles. Skin sensitization may also occur. Eye contact may result in conjunctivitis and corneal injury. Kidney and liver damage may occur. Vomiting may also occur. Exposure to this type of compound can cause central nervous system stimulation, vomiting, diarrhea, paresthesia, excitement, giddiness, fatigue, tremors, convulsions, coma, pulmonary edema, hypothermia and liver, kidney and myocardial toxicity. Respiration may be initially accelerated and then later depressed. Chronic exposure to this type of compound leads to headache, loss of appetite, muscular weakness, fine tremors and apprehensive mental state. **ACUTE/CHRONIC HAZARDS:** This compound is harmful if swallowed, inhaled or absorbed through the skin. It may cause irritation. When heated to decomposition it emits toxic fumes of chlorine, carbon monoxide, carbon dioxide, nitrogen oxides, hydrogen chloride gas and phosgene. (NTP, 1992)

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

Gastrointestinal decontamination. If a large amount of the fungicide has been ingested in the last few hours, and if copious vomiting has not already occurred, it may be reasonable to consider GI decontamination. Activated charcoal can be used along with the addition of the cathartic sorbitol to the charcoal slurry. If sorbitol is given separately, it should be diluted with an equal volume of water before administration. No more than one dose of sorbitol is recommended and it should be used with caution in children and the elderly. If contact with the toxicant has been minimal (for example, oral contamination only, promptly flushed out of the mouth), administration of charcoal without a cathartic, followed by careful observation of the patient, probably represents optimal management. Substituted benzenes

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

This chemical is a combustible solid. Use dry chemical, carbon dioxide, water spray, or alcohol foam extinguishers. Poisonous gases are produced in fire. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Notify local health and fire officials and pollution control agencies. From a secure, explosion-proof location, use water spray to cool exposed containers. If cooling streams are ineffective (venting sound increases in volume and pitch, tank discolors, or shows any signs of deforming), withdraw immediately to a secure position. If employees are expected to fight fires, they must be trained and equipped in OSHA 1910.156

5.2 Specific hazards arising from the chemical

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

5.3 Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media.

SECTION 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. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: particulate filter respirator adapted to the airborne concentration of the substance.

6.3 Methods and materials for containment and cleaning up

This pesticide is toxic to birds and mammals. Treated seed and granules on soil surface may be hazardous to terrestrial wildlife. Cover or collect any such materials spilled during loading.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

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

Provision to contain effluent from fire extinguishing. Store in a refrigerator or cool, dry place away from strong bases. A regulated, marked area should be established where this chemical is handled, used, or stored in compliance with OSHA standard 1910.1045.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

TLV: 0.5 mg/m³, as TWA; A4 (not classifiable as a human carcinogen)

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

Avoid inhalation of dust.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	PHYSICAL DESCRIPTION: Crystalline pale yellow to white solid or powder with a musty moth ball odor. Insoluble in water and denser than water. Hence sinks in water.
Colour	Pale yellow crystals
Odour	Musty odor
Melting point/freezing point	144°C
Boiling point or initial boiling point and boiling range	328°C
Flammability	Liquid formulations containing organic solvents may be flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	11°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 1 mg/mL at 72° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 4.22
Vapour pressure	0.013 mm Hg at 77° F (NTP, 1992)
Density and/or relative density	1.718
Relative vapour density	10.2 (NTP, 1992) (Relative to Air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Decomposes on heating. This produces toxic and corrosive fumes including chlorides and nitrogen oxides. Decomposes on heating. This produces toxic gases of nitrogen oxides, hydrogen chloride, phosgene and chlorine. The substance is a strong oxidant. It reacts violently with combustible and reducing materials.

10.2 Chemical stability

Stable in sunlight

10.3 Possibility of hazardous reactions

QUINTOZONE is hydrolyzed by alkalis. Is incompatible with strong oxidizing agents. Also incompatible with strong bases. Corrosive to unlined metal containers (NTP, 1992).

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Alkalies

10.6 Hazardous decomposition products

When heated to decomposition, it emits highly toxic fumes of chlorides and oxides of nitrogen.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral greater than 12000 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

Cancer Classification: Group C Possible Human Carcinogen

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

The substance may have effects on the liver. This may result in impaired functions.

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50; Species: *Lepomis macrochirus* (Bluegill); Conditions: freshwater, flow through; Concentration: 0.1 ppm for 96 hr (95% confidence interval: 0.092-0.14 ppm) /98.2% purity
- Toxicity to daphnia and other aquatic invertebrates: EC50; Species: *Daphnia magna* (Water flea, first instar larvae); Conditions: freshwater, static; Concentration: 0.77 ppm for 48 hr (95% confidence interval: 0.62-1.1 ppm); Effect: intoxication, immobilization
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC/SLUDGE: After 5 days incubation with activated sludge as the seed and at an initial concentration of 50 ug/L, 7.0% of the pentachloronitrobenzene was mineralized to CO₂(1). In an aerobic screening test using an activated sludge inoculum, a half-life of 4.3 days was measured for pentachloronitrobenzene at 100 ug/L(2). Less than 0.1% of the initial pentachloronitrobenzene in a 5 day aqueous screening test was biodegraded by an activated sludge inoculum(3).

12.3 Bioaccumulative potential

Measured bioconcentration factors for pentachloronitrobenzene in fish are 238 (topmouth gudgeon, 14 day continuous flow test, compound present at 5-20 ppb)(1), 1,140 (golden orfe, 3 day static test)(2) and 114-261 (rainbow trout; compound concentration of 690 ng/L; flow-through test duration of 5-36 days)(3). BCF values for pentachloronitrobenzene in golden orfe were 430, 950, and 1,130;

however, the toxicity limit was exceeded for the first two BCF values and only 70% of the initial radioactivity was recovered from the fish and water for the latter BCF, indicating that some of the pentachloronitrobenzene was lost(4). According to a classification scheme(5), these BCF values suggest the potential for bioconcentration in aquatic organisms is high(SRC). Other BCF values for pentachloronitrobenzene were 14,000 and 22,000 (algae)(4), 4,508 (Chlorella fusca)(6) and 4,500 (activated sludge)(4).

12.4 Mobility in soil

A Koc of 21,877 was measured according to OECD TG 106 protocol using a Podsol and an Alfisol(1). A Koc of 19,000 has also been reported, test conditions not specified(2) According to a recommended classification scheme(3), these Koc values indicate that pentachloronitrobenzene will be immobile in soil, particularly those soils containing high concentrations of organic matter(SRC). Analyses of soil samples collected at the groundwater level from cultivated land treated frequently with pentachloronitrobenzene confirmed that this compound is not transported below a depth greater than plow layer(4). Evaporation and movement of pentachloronitrobenzene is strongly inhibited by higher organic matter content of soil(4).

12.5 Other adverse effects

no data available

SECTION 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.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN3077 (For reference only, please check.) IMDG: UN3077 (For reference only, please check.) IATA: UN3077 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.) IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.) IATA: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 9 (For reference only, please check.) IMDG: 9 (For reference only, please check.) IATA: 9 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: III (For reference only, please check.) IMDG: III (For reference only, please check.) IATA: III (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes IMDG: Yes IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Quintozene	Quintozene	82-68-8	201-435-0
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			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)	Not Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2019
Revision Date August 08, 2025

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

If the substance is formulated with solvent(s) also consult the card(s) (ICSC) of the solvent(s). Carrier solvents used in commercial formulations may change physical and toxicological properties.

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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.