

## SECTION 1: CHEMICAL PRODUCT and COMPANY IDENTIFICATION

Catalog No.  
L03045

**Product Name:** Pentachloronitrobenzene, 99%  
**Synonyms:** Nitropentachlorobenzene

**Manufacturer/Supplier Name:** Alfa Aesar - A Johnson Matthey Company  
**Address:** 30 Bond St.  
Ward Hill, MA 01835

**Business Phone:** 978-521-6300  
**Business Fax:** 978-521-6350

**For information in North America, call:** 978-521-6300

**CHEMTREC Numbers:**

**For emergencies in the US, call CHEMTREC: 800-424-9300**  
**For emergencies outside US, call INTERNATIONAL: (703)527-3887**  
**For Nonemergency, call: (800)262-8200**

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## SECTION 2 : COMPOSITION, INFORMATION ON INGREDIENTS

Catalog No. L03045

<b>Chemical Name</b>	Pentachloronitrobenzene
<b>CAS#</b>	82-68-8
<b>% Weight (Typical)</b>	99

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## SECTION 3 : HAZARDS IDENTIFICATION

Catalog No. L03045

**Emergency Overview:** Highly toxic. Sensitizer. Reproductive effects. Mutation data.

**Pentachloronitrobenzene:**

**Route of Exposure:** Skin. Inhalation. Ingestion.

**Potential Health Effects:**

**Eye Contact:** No data

**Skin Contact:** Possible skin sensitiser.

**Inhalation:** Highly Toxic by inhalation.

**Ingestion:** Harmful if swallowed.

**Target Organs:** Skin. Respiratory system. G.I. Tract. Reproductive System.

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**SECTION 4 : FIRST AID MEASURES**Catalog No. L03045

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<b>Eye Contact:</b>	Immediately flush eyes with plenty of water for at least 20 minutes. Assure adequate flushing of the eyes by separating the eyelids with fingers. Get immediate medical attention if irritation persists, or symptoms of overexposure become apparent.
<b>Skin Contact:</b>	Immediately wash skin with plenty of water for at least 20 minutes, while removing contaminated clothing and shoes. Get medical attention especially, if irritation develops, persists, or symptoms of overexposure become apparent.
<b>Inhalation:</b>	Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Keep warm. Get immediate medical attention.
<b>Ingestion:</b>	If swallowed, call a physician or poison control center immediately. Never give anything by mouth to an unconscious person. Do not induce vomiting unless instructed by medical personnel. Get medical attention.

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**SECTION 5 : FIRE FIGHTING MEASURES**Catalog No. L03045

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<b>Flash Point:</b>	No data
<b>Extinguishing Media:</b>	Use dry powder or carbon dioxide when fighting a fire involving this material.
<b>Unsuitable Media:</b>	Water extinguishers are not recommended.
<b>Protective Equipment:</b>	As in any fire, wear self-contained breathing apparatus pressure-demand, NIOSH (approved or equivalent) and full protective gear.

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**SECTION 6 : ACCIDENTAL RELEASE MEASURES**Catalog No. L03045

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<b>Personal Precautions:</b>	Use proper personal protective equipment as listed in section 8.
<b>Spill Cleanup Measures:</b>	Clean up spills immediately, observing precautions in the Protective Equipment section. Sweep up or absorb material, then place into a suitable clean, dry, closed container. Avoid generating dusty conditions. Refer to section 13 for disposal requirements.
<b>Environmental Precautions:</b>	Do not allow material to enter drains or streams.

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**SECTION 7 : HANDLING and STORAGE**Catalog No. L03045

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<b>Handling:</b>	This product should be handled only by, or under the close supervision of, those properly qualified in the handling and use of potentially hazardous chemicals, who should take into account the fire, health and chemical hazard data. It should always be handled in an efficient fume hood or equivalent system. The user should consider that the toxicological and physiological properties of many compounds are not yet well determined and that new hazardous products may arise from reactions between chemicals. Care should be taken to prevent any chemical from coming into contact with the skin or eyes and from contaminating personal clothing.
<b>Storage:</b>	Store in a cool, dry, well ventilated area away from sources of heat and incompatible substances. Keep container tightly closed when not in use.
<b>Hygiene Practices:</b>	Wash thoroughly after handling. Avoid contact with eyes and skin. Avoid inhaling dust.

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**SECTION 8 : EXPOSURE CONTROLS, PERSONAL PROTECTION**Catalog No. L03045

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Guideline Type: ACGIH TLV-TWA

Guideline Information: 0.5 mg/m3

**Engineering Controls:** Use appropriate engineering control such as process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits. Where such systems are not effective wear suitable personal protective equipment, which performs satisfactorily and meets OSHA or other recognized standards. Consult with local procedures for selection, training, inspection and maintenance of the personal protective equipment.

**Skin Protection Description:** Wear suitable protective clothing to prevent contact with skin.

**Hand Protection Description:** Wear appropriate protective gloves. Consult glove manufacturers for glove permeability data.

**Eye/Face Protection:** Wear appropriate protective glasses or splash goggles as described by 29 CFR 1910.133, OSHA eye and face protection regulation, or the European standard EN 166.

**Respiratory Protection:** A NIOSH approved air-purifying respirator with an appropriate cartridge or canister may be permissible under certain circumstances where airborne concentrations are expected to exceed exposure limits. Protection provided by air purifying respirators is limited to airborne concentrations that are typically within 10 times the exposure limit. Use a positive pressure air supplied respirator if there is any potential for an uncontrolled release, exposure levels are not known, or any other circumstances where air-purifying respirators may not provide adequate protection. A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements must be followed whenever workplace conditions warrant a respirators use.

**Other Protective:** Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower.

**Ingredient Guidelines**Ingredient: Pentachloronitrobenzene[To Top of page](#)

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**SECTION 9 : PHYSICAL and CHEMICAL PROPERTIES**Catalog No. L03045

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**Physical State/Appearance:** Solid

**Color:** Cream to pale yellow

**Flash Point:** No data

**Boiling Point:** 328°C (622.4°F)

**Melting Point:** 140-143°C (284-289.4°F)

**n-Octanol/water partition coefficient:** 4.22

**Solubility in Water:** 0.001 g/L @ 25°C (77°F)

**Density:** No data

**Molecular Formula:** C<sub>6</sub>Cl<sub>5</sub>NO<sub>2</sub>

**Molecular Weight:** 295.34

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**SECTION 10 : STABILITY and REACTIVITY**Catalog No. L03045

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**Conditions to Avoid:** Heat, flames and sparks.

**Incompatibilities with Other Materials:** Oxidizing agents.

**Possible Decomposition Product:** Hydrogen cyanide, oxides of nitrogen. Hydrogen chloride.

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**SECTION 11 : TOXICOLOGICAL INFORMATION**Catalog No. L03045

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**Pentachloronitrobenzene :**

<b>RTECS Number:</b>	DA6650000
<b>Eye Effect:</b>	No data reported in the cited references as of the revision date.
<b>Skin Effects:</b>	Skin - rabbit LD50: >4 gm/kg (Supplier data)
<b>Ingestion Effects:</b>	Oral - rat LD50: 1100 mg/kg (RTECS); Oral - mouse LD50: 1400 mg/kg (RTECS); Oral - rabbit LD50: 800 mg/kg (RTECS)
<b>Inhalation Effects:</b>	Inhalation - rat LC50: 1400 mg/m <sup>3</sup> (RTECS); Inhalation -mouse LC50: 2 gm/m <sup>3</sup> (RTECS)
<b>Chronic Ingestion Effects:</b>	Oral - rat TDLo: 11250 mg/kg/90D-C Liver - changes in liver weight Kidney, Ureter, Bladder - changes in bladder weight Nutritional and Gross Metabolic - weight loss or decreased weight gain (RTECS); Oral -mouse TDLo: 13650 mg/kg/13W-I Liver - changes in liver weight (RTECS)
<b>Carcinogenicity:</b>	IARC-3 Carcinogen - Unclassifiable as to Carcinogenicity in Humans. ACGIH TLV-A4 - Not Classifiable as a Human Carcinogen. Carcinogenic by RTECS criteria.
<b>Mutagenicity:</b>	Mutation data reported. (RTECS).
<b>Teratogenicity:</b>	Teratogenic effects. (RTECS)
<b>Reproductive Toxicity:</b>	Reproductive effects. (RTECS)
<b>Other Toxicological Information:</b>	Intraperitoneal - rat LD50: 5 gm/kg; Intraperitoneal - mouse LD50: 4500 mg/kg

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**SECTION 12 : ECOLOGICAL INFORMATION**Catalog No. L03045

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<b>Ecotoxicity:</b>	No data. May cause long term affects in the environment.
<b>Bioaccumulation:</b>	Potential for bioaccumulation is high.
<b>Biodegradation:</b>	Not expected to be biodegradable. Very slow to photodegrade in the atmosphere, half-life ca 2200 days.
<b>Environmental Stability:</b>	No information provided.

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**SECTION 13 : DISPOSAL CONSIDERATIONS**Catalog No. L03045

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<b>Waste Disposal:</b>	Consult with the US EPA Guidelines listed in 40 CFR Part 261.3 for the classifications of hazardous waste prior to disposal. Furthermore, consult with your state and local waste requirements or guidelines, if applicable, to ensure compliance. Arrange disposal in accordance to the EPA and/or state and local guidelines, by a licensed disposal company.
<b>EPA Waste Number:</b>	U185 for Pentachloronitrobenzene CAS Number: 82-68-8

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**SECTION 14 : TRANSPORT INFORMATION**Catalog No. L03045

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<b>DOT Shipping Name:</b>	Aviation regulated solid, n.o.s.
<b>DOT Hazard Class:</b>	9
<b>DOT Identification Number:</b>	UN3335

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**Pentachloronitrobenzene :**

**TSCA 8(b): Inventory Status:** Listed on the TSCA inventory.

**Risk Phrases:** R43 May cause sensitization by skin contact.

**Safety Phrase:** S24 Avoid contact with skin.  
S37 Wear suitable gloves.

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## SECTION 16 : ADDITIONAL INFORMATION

**MSDS Preparation Date:** January 1, 2002, Version 1

**MSDS Revision Date:** April 14, 2003.

**MSDS Author:** Actio Corporation.

**Disclaimer:**

This Health and Safety Information is correct to the best of our knowledge and belief at the date of its publication but we cannot accept liability for any loss, injury or damage which may result from its use. We shall ensure, so far as is reasonably practicable, that any revision of this Data Sheet is sent to all customers to whom we have directly supplied this substance, but must point out that it is the responsibility of any intermediate supplier to ensure that such revision is passed to the ultimate user. The information given in the Data Sheet is designed only as a guidance for safe handling, storage and the use of the substance. It is not a specification nor does it guarantee any specific properties. All chemicals should be handled only by competent personnel, within a controlled environment. Should further information be required, this can be obtained through the sales office whose address is at the top of this data sheet. We welcome any additional information about our products that customers have obtained by personal experience.

**References:**

1. American Chemical Society, STN Easy Online Database
2. Brethericks Reactive Chemical Hazards Database. Version 2.
3. Gassarett and Doulls Toxicology, The Basic Science of Poisons.
4. Hawleys Condensed Chemical Dictionary, Thirteenth Edition
5. IARC monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man, WHO International Research on Cancer.
6. Industrial Hygiene and Toxicology, by F.A. Patty.
7. National Library of Medicine, Department of Health and Human Services, Hazardous Substances Data Bank (HSDB).
8. National Toxicology Program (NTP) Eighth Report on Carcinogens, 1997.
9. NIOSH Registry of Toxic Effects of Chemical Substances (RTECS) and Pocket Guide to Chemical Hazards.
10. OSHA Hazard Communication Standard, 1910.1200 and Z Tables.
11. Sax Dangerous Properties of Industrial Materials. Tenth Edition.
12. The Merck Index: An Encyclopedia of Chemicals and Drugs. Merck and Company. Twelfth Edition 1998.
13. Threshold Limit Values for Chemical Substances and Physical Agents in the Work Environmental and Biological Exposure Indices. TLV Booklet, 2001.