

SAFETY DATA SHEET

Version 6.13
Revision Date 04/30/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 5-Chloro-2-nitrobenzaldehyde
Product Number : C58800
Brand : Aldrich
CAS-No. : 6628-86-0

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

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Corrosive to Metals : Category 1
Acute toxicity (Oral) : Category 4

Skin irritation : Category 2
Serious eye damage : Category 1
Skin sensitization : Category 1
Short-term (acute) aquatic hazard : Category 1
Long-term (chronic) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal Word : Danger

Hazard Statements : H290 May be corrosive to metals.
H302 Harmful if swallowed.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements : **Prevention:**
P234 Keep only in original container.
P261 Avoid breathing dust.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P272 Contaminated work clothing must not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
Response:
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P390 Absorb spillage to prevent material damage.
P391 Collect spillage.

Storage:

P406 Store in corrosive resistant container with a resistant inner liner.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
5-Chloro-2-nitrobenzaldehyde	6628-86-0*	>= 70 - < 90	-
3-Chloro-4-nitrobenzaldehyde	57507-34-3*	>= 10 - < 20	-
5-chloro-2-nitrobenzoic acid	2516-95-2*	>= 5 - < 10	-
sulphuric acid	7664-93-9*	>= 1 - < 5	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this material safety data sheet to the doctor in attendance.
If inhaled : After inhalation: fresh air.
In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact : After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed : After swallowing: immediately make victim drink water (two glasses at most).

Consult a physician.

Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media : Water
Foam
Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

Sulfur oxides

Hydrogen chloride gas

Specific extinguishing methods : No data available

Further information : Suppress (knock down) gases/vapors/mists with a water spray jet.
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective : Stay in danger area only with self-contained breathing

equipment for fire-fighters

apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Avoid inhalation of dusts.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.
- Environmental precautions : Do not let product enter drains.
- Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Conditions for safe storage : No metal containers.
- Further information on storage conditions : Tightly closed.
Dry.
- Storage class : 8A, Combustible, corrosive hazardous materials
- Recommended storage temperature : Recommended storage temperature see product label.
- Packaging material : Suitable material: Amber Glass Bottle/Jar

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
sulphuric acid	7664-93-9	TWA	1 mg/m ³	NIOSH REL

		TWA (Thoracic particulate matter)	0.2 mg/m ³	ACGIH
		TWA	1 mg/m ³	OSHA Z-1
		TWA	1 mg/m ³	OSHA P0

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : Nitrile rubber
 Break through time : 480 min
 Glove thickness : 0.11 mm
 Protective index : Full contact
 Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
 Break through time : 480 min
 Glove thickness : 0.11 mm
 Protective index : Splash contact
 Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.
 This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Tightly fitting safety goggles
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : powder
- Color : light red
- Odor : No data available
- Odor Threshold : No data available
pH : No data available
- Melting point/ range : 149 - 156 °F / 65 - 69 °C
Method: lit.
- Boiling point/boiling range : No data available
- Flash point : No data available
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Upper explosion limit /
Upper flammability limit : No data available
- Lower explosion limit /
Lower flammability limit : No data available
- Vapor pressure : No data available
- Relative vapor density : No data available
- Relative density : No data available

Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: log Pow: 2.077
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 185.56 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: no information available
Incompatible materials	: Strong bases
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Acute toxicity estimate Oral - 715.65 mg/kg
(Calculation method)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

3-Chloro-4-nitrobenzaldehyde:

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Toxicity to fish : Remarks: No data available

5-chloro-2-nitrobenzoic acid:

Toxicity to fish : Remarks: No data available

LC50 : 0.616 mg/l
Exposure time: 96.0 h

LC50 : 0.1 mg/l
Exposure time: 96.0 h

M-Factor (Acute aquatic toxicity) : 10

sulphuric acid:

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): > 100 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Desmodesmus subspicatus (green algae)): > 100 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

Ecotoxicology Assessment

Acute aquatic toxicity : This product has no known ecotoxicological effects.

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

3-Chloro-4-nitrobenzaldehyde:

Biodegradability : Remarks: No data available

5-chloro-2-nitrobenzoic acid:

Biodegradability : Remarks: No data available

sulphuric acid:

Biodegradability : Remarks: The methods for determining the biological

degradability are not applicable to inorganic substances.

Bioaccumulative potential

Components:

5-Chloro-2-nitrobenzaldehyde:

Partition coefficient: n- : log Pow: 2.077
octanol/water Remarks: Bioaccumulation is not expected.

3-Chloro-4-nitrobenzaldehyde:

Bioaccumulation : Remarks: No data available

5-chloro-2-nitrobenzoic acid:

Bioaccumulation : Remarks: No data available

sulphuric acid:

Partition coefficient: n- : Remarks: Not applicable for inorganic substances
octanol/water

Mobility in soil

Components:

5-Chloro-2-nitrobenzaldehyde:

Stability in soil : Remarks: No data available

3-Chloro-4-nitrobenzaldehyde:

Stability in soil : Remarks: No data available

5-chloro-2-nitrobenzoic acid:

Stability in soil : Remarks: No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

3-Chloro-4-nitrobenzaldehyde:

Additional ecological information : No data available

sulphuric acid:

Results of PBT and vPvB assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

Additional ecological information : Biological effects:

Harmful effect due to pH shift.

Caustic even in diluted form.

Does not cause biological oxygen deficit.

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Neutralisation possible in waste water treatment plants.

Discharge into the environment must be avoided.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1759
Proper shipping name : Corrosive solid, n.o.s.
(sulphuric acid)
Class : 8
Packing group : III
Labels : Class 8 - Corrosive substances
Packing instruction (cargo aircraft) : 864
Packing instruction (passenger aircraft) : 860

IMDG-Code

UN number : UN 1759
 Proper shipping name : CORROSIVE SOLID, N.O.S.
 (sulphuric acid)
 Class : 8
 Packing group : III
 Labels : 8
 EmS Code : F-A, S-B
 Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation**49 CFR Road**

UN/ID/NA number : UN 1759
 Proper shipping name : Corrosive solids, n.o.s.
 (sulphuric acid)
 Class : 8
 Packing group : III
 Labels : Class 8 - Corrosive substances
 ERG Code : 154
 Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION**CERCLA Reportable Quantity**

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

SARA 304 Extremely Hazardous Substances Reportable Quantity

Listed substances in the product are at low enough levels to not be expected to exceed the RQ

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
sulphuric acid	7664-93-9	1000

SARA 311/312 Hazards : Acute Health Hazard
 Chronic Health Hazard

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA P0	:	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
OSHA P0 / TWA	:	8-hour time weighted average
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and

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Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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