

## 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.

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### 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

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### 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).

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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

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## SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media : Water  
Foam  
Carbon dioxide (CO<sub>2</sub>)  
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<sub>x</sub>)

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.

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## 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.

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## 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

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

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

|  |  |                                            |                       |          |
|--|--|--------------------------------------------|-----------------------|----------|
|  |  | TWA<br>(Thoracic<br>particulate<br>matter) | 0.2 mg/m <sup>3</sup> | ACGIH    |
|  |  | TWA                                        | 1 mg/m <sup>3</sup>   | OSHA Z-1 |
|  |  | TWA                                        | 1 mg/m <sup>3</sup>   | 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 Dermatrill® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatrill® 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](http://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).<br>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.                                   |

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## 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<br>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 /<br>Upper flammability limit | : No data available                         |
| Lower explosion limit /<br>Lower flammability limit | : No data available                         |
| Vapor pressure                                      | : No data available                         |
| Relative vapor density                              | : No data available                         |
| Relative density                                    | : No data available                         |

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|                                           |                                |
|-------------------------------------------|--------------------------------|
| 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<br>Particle size | : No data available            |

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## 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                                                                                                                                                       |



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## 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

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## 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-octanol/water : log Pow: 2.077  
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-octanol/water : Remarks: Not applicable for inorganic substances

### **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.

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## 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.

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## 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.

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**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

**SARA 313**

: The following components are subject to reporting levels established by SARA Title III, Section 313:

sulphuric acid      7664-93-9       $\geq 1 - < 5 \%$

**Clean Air Act**

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).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

**Clean Water Act**

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

sulphuric acid      7664-93-9       $\geq 1 - < 5 \%$

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

sulphuric acid      7664-93-9       $\geq 1 - < 5 \%$

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

**US State Regulations****Massachusetts Right To Know**

sulphuric acid      7664-93-9

**Pennsylvania Right To Know**

sulphuric acid      7664-93-9

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**California Prop. 65**

WARNING: This product can expose you to chemicals including sulphuric acid, which is/are known to the State of California to cause cancer. For more information go to [www.P65Warnings.ca.gov](http://www.P65Warnings.ca.gov).

**The ingredients of this product are reported in the following inventories:**

TSCA      : Product contains substance(s) not listed on TSCA inventory.

## TSCA list

No substances are subject to a Significant New Use Rule.

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

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## 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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