1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name: 4-Nitroaniline

Product Number: 31569
Brand: Sigma-Aldrich
Index-No.: 612-012-00-9

CAS-No.: 100-01-6

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103 USA

Telephone: +1 800-325-5832
Fax: +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone #: (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - repeated exposure (Category 2), H373
Acute aquatic toxicity (Category 3), H402
Chronic aquatic toxicity (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s)
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled
H373 May cause damage to organs through prolonged or repeated exposure.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)
P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing.
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P302 + P352 + P312 IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor if you feel unwell.
P304 + P340 + P311 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician.
P314 Get medical advice/attention if you feel unwell.
P361 Remove/Take off immediately all contaminated clothing.
P363 Wash contaminated clothing before reuse.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₆H₆N₂O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>138.12 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>100-01-6</td>
</tr>
<tr>
<td>EC-No.</td>
<td>202-810-1</td>
</tr>
<tr>
<td>Index-No.</td>
<td>612-012-00-9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-Nitroaniline</td>
<td>Acute Tox. 3; STOT RE 2; Aquatic Acute 3; Aquatic Chronic 3; H301 + H311 + H331, H373, H412</td>
<td>&lt;= 100%</td>
</tr>
</tbody>
</table>

For the full text of the H-Stations mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

**General advice**
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**
Flush eyes with water as a precaution.

**If swallowed**
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 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.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.
5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.
Moisture sensitive.
Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-Nitroaniline</td>
<td>100-01-6</td>
<td>TWA</td>
<td>3.000000 mg/m³</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td>Remarks</td>
<td></td>
<td></td>
<td></td>
<td>Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers</td>
</tr>
</tbody>
</table>

Sigma-Aldrich - 31569
Not classifiable as a human carcinogen
Danger of cutaneous absorption

<table>
<thead>
<tr>
<th>TWA</th>
<th>USA. NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.000000 mg/m3</td>
<td></td>
</tr>
</tbody>
</table>

Potential for dermal absorption

<table>
<thead>
<tr>
<th>TWA</th>
<th>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000000 ppm</td>
<td>6.000000 mg/m3</td>
</tr>
</tbody>
</table>

Skin designation
The value in mg/m3 is approximate.

<table>
<thead>
<tr>
<th>PEL</th>
<th>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 mg/m3</td>
<td></td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: crystalline
   Colour: yellow

b) Odour
   Ammonia odor

b) Odour Threshold
   No data available

d) pH
   7.0

e) Melting point/freezing point
   Melting point/range: 146 - 149 °C (295 - 300 °F) - lit.

f) Initial boiling point and boiling range
   260 °C (500 °F) at 133 hPa (100 mmHg) - lit.

g) Flash point
   213.0 °C (415.4 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapour pressure
   0.005 hPa (0.004 mmHg) at 25.0 °C (77.0 °F)

l) Vapour density
   No data available

m) Relative density
   1.44 g/cm3

n) Water solubility
   slightly soluble

o) Partition coefficient: n-octanol/water
   log Pow: 1.39

p) Auto-ignition temperature
   180.0 °C (356.0 °F)

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   No data available

9.2 Other safety information

Bulk density
   630 kg/m3

10. STABILITY AND REACTIVITY

10.1 Reactivity
   No data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   No data available

10.4 Conditions to avoid
   No data available

10.5 Incompatible materials
   Strong acids, Strong oxidizing agents, Strong reducing agents, Plastics, Rubber

10.6 Hazardous decomposition products
   Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)
11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 750.0 mg/kg
LD50 Dermal - Guinea pig - > 500.0 mg/kg
No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available
Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard
No data available

Additional Information
RTECS: BY7000000
Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer. Exposure to and/or consumption of alcohol may increase toxic effects. Headache, Unconsciousness, Cough, chest pain, Difficulty in breathing, Drowsiness, Nausea, Cyanosis, Ataxia, Diarrhoea, Vomiting. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. p-Nitroaniline is readily absorbed by inhalation, ingestion, or skin absorption. It is a strong methemoglobin former. Cyanosis is the first manifestation of toxicity.
Liver -

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish
LC50 - Pimephales promelas (fathead minnow) - 85.7 - 142 mg/l - 96.0 h
LC50 - Leuciscus idus (Golden orfe) - 35 mg/l - 48.0 h
LC50 - Danio rerio (zebra fish) - 87.6 mg/l - 96.0 h
Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 17.00 mg/l - 48 h

Toxicity to algae

EC50 - No information available. - 68.00 mg/l - 24 h

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

Bioaccumulation

Danio rerio (zebra fish) - 96 h
- 0.028 mg/l

Bioconcentration factor (BCF): 4.4

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1661 Class: 6.1 Packing group: II
Proper shipping name: Nitroanilines
Reportable Quantity (RQ): 5000 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 1661 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: NITROANILINES (o-, m-, p-)

IATA

UN number: 1661 Class: 6.1 Packing group: II
Proper shipping name: Nitroanilines

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

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

<table>
<thead>
<tr>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-Nitroaniline</td>
<td>100-01-6</td>
</tr>
</tbody>
</table>

SARA 311/312 Hazards

Acute Health Hazard
Massachusetts Right To Know Components

p-Nitroaniline

CAS-No. 100-01-6
Revision Date 2007-07-01

Pennsylvania Right To Know Components

p-Nitroaniline

CAS-No. 100-01-6
Revision Date 2007-07-01

New Jersey Right To Know Components

p-Nitroaniline

CAS-No. 100-01-6
Revision Date 2007-07-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity
Aquatic Acute Acute aquatic toxicity
Aquatic Chronic Chronic aquatic toxicity
H301 Toxic if swallowed.
H301 + H311 + Toxic if swallowed, in contact with skin or if inhaled
H331
H311 Toxic in contact with skin.
H331 Toxic if inhaled.

HMIS Rating
Health hazard: 2
Chronic Health Hazard:
Flammability: 1
Physical Hazard 0

NFPA Rating
Health hazard: 2
Fire Hazard: 1
Reactivity Hazard: 0

Further information
Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling
or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.6 Revision Date: 05/24/2016 Print Date: 08/03/2016