1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name: 3-Phenoxyphenylacetonitrile
Product Number: 357766
Brand: Aldrich
CAS-No.: 51632-29-2

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 Inc.
3050 Spruce Street
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
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 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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: CUST-N15.00700530

Hazard statement(s)
H302 + H312 + H332  Harmful if swallowed, in contact with skin or if inhaled.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H335  May cause respiratory irritation.

Precautionary statement(s)
P261  Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

| Formula | C_{14}H_{11}NO |
| Molecular weight | 209.24 g/mol |
| CAS-No. | 51632-29-2 |

Hazardous components

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-Phenoxyphenylacetonitrile</td>
<td>Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H302 + H312 + H332, H315, H319, H335</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements 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. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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
Carbon oxides, Nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)

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
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. 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 inhalation of vapour or mist.
Normal measures for preventive fire protection.
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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): 10: Combustible liquids

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

<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>3-Phenoxyphenylacetonitrile</td>
<td>51632-29-2</td>
<td>TWA</td>
<td>5.000000 mg/m3</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
</tbody>
</table>

Remarks: CAS number varies with compound
Skin designation: C

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.700000 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.000000 mg/m3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

10 minute ceiling value
Upper Respiratory Tract irritation
Headache
Nausea
Thyroid effects
Danger of cutaneous absorption varies

TWA 5 mg/m³ USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

CAS number varies with compound
Skin designation

C 5 mg/m³ USA. ACGIH Threshold Limit Values (TLV)

Upper Respiratory Tract irritation
Headache
Nausea
Thyroid effects
Danger of cutaneous absorption varies

C 4.7 ppm USA. NIOSH Recommended Exposure Limits

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: liquid
   Colour: light yellow

b) Odour
   No data available

c) Odour Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   No data available

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>5.000000 mg/m³</th>
<th>USA. ACGIH Threshold Limit Values (TLV)</th>
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<tr>
<td></td>
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<thead>
<tr>
<th></th>
<th>C</th>
<th>4.7 ppm</th>
<th>USA. NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
</table>
f) Initial boiling point and boiling range 137 °C (279 °F) at 0.4 hPa - lit.
g) Flash point 113 °C (235 °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 No data available
l) Vapour density No data available
m) Relative density 1.124 g/cm³ at 25 °C (77 °F)
n) Water solubility No data available
o) Partition coefficient: n-octanol/water No data available
p) Auto-ignition temperature No data available
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
No data available

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 oxidizing agents
10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects
Acute toxicity
LD50 Intraperitoneal - Mouse - 105 mg/kg
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

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: AM1370000

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness

Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available(3-Phenoxyphenylacetonitrile)

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
No data available
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)
Not dangerous goods

IMDG
Not dangerous goods

IATA
UN number: 3334 Class: 9 Packing group: III
Proper shipping name: Aviation regulated liquid, n.o.s. (3-Phenoxyphenylacetonitrile)

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
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

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

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-Phenoxyphenylacetonitrile</td>
<td>51632-29-2</td>
<td>2010-08-02</td>
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New Jersey Right To Know Components

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California Prop. 65 Components

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<tbody>
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<td>3-Phenoxyphenylacetonitrile</td>
<td>51632-29-2</td>
<td>2013-07-26</td>
</tr>
</tbody>
</table>

16. OTHER INFORMATION

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

H302 Harmful if swallowed.
H302 + H312 + Harmful if swallowed, in contact with skin or if inhaled.
H332
H312 Harmful in contact with skin.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H332 Harmful if inhaled.
H335 May cause respiratory irritation.

**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**
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**Preparation Information**
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956
Version: 6.0 Revision Date: 11/06/2017 Print Date: 11/21/2018