**SECTION 1: Identification of the substance/mixture and of the company/undertaking**

1.1 **Product identifiers**

- **Product name**: 1,3-Dinitrobenzene
- **Product Number**: 45966
- **Brand**: Sigma-Aldrich
- **Index-No.**: 609-004-00-2
- **CAS-No.**: 99-65-0

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 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**

2.1 **Classification of the substance or mixture**

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

- Acute toxicity, Oral (Category 2), H300
- Acute toxicity, Inhalation (Category 2), H330
- Acute toxicity, Dermal (Category 1), H310
- Specific target organ toxicity - repeated exposure (Category 2), H373
- Short-term (acute) aquatic hazard (Category 1), H400
- Long-term (chronic) aquatic hazard (Category 1), H410

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)
H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.
H373 May cause damage to organs through prolonged or repeated exposure.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)
P260 Do not breathe dust.
P262 Do not get in eyes, on skin, or on clothing.
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.
P284 Wear respiratory protection.
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P314 Get medical advice/ attention if you feel unwell.
P362 Take off contaminated clothing and wash before reuse.
P391 Collect spillage.
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

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Dinitrobenzene</td>
<td>Acute Tox. 2; Acute Tox. 1; STOT RE 2; Aquatic Acute 1; Aquatic Chronic 1, H300, H330, H310, H373, H400, H410</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Sigma-Aldrich - 45966
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

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

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

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.
5.3 **Advice for firefighters**  
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **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.

### SECTION 6: Accidental release measures

6.1 **Personal precautions, protective equipment and emergency procedures**  
Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. 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**  
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 **Reference to other sections**  
For disposal see section 13.

### SECTION 7: Handling and storage

7.1 **Precautions for safe handling**  
**Advice on safe handling**  
Work under hood. Do not inhale substance/mixture.

**Hygiene measures**  
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**  
**Storage conditions**  
Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage class**  
Storage class (TRGS 510): 6.1A: 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.
SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients 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>m-Dinitrobenzene</td>
<td>99-65-0</td>
<td>TWA</td>
<td>1 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
</tbody>
</table>

Remarks: Potential for dermal absorption

<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>m-Dinitrobenzene</td>
<td>99-65-0</td>
<td>TWA</td>
<td>1 mg/m3</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
</tbody>
</table>

Skin designation

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Dinitrobenzene</td>
<td>99-65-0</td>
<td>Methemoglobin</td>
<td>5% Hb</td>
<td>In blood</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Dinitrobenzene</td>
<td>99-65-0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Remarks: During or at the end of the shift

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

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

Skin protection
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).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min  
Material tested: KCL 741 Dermatril® L

Splash contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: KCL 741 Dermatril® L

**Body Protection**  
Protective clothing

**Respiratory protection**  
Recommended Filter type: Filter type P3

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.

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.

**Control of environmental exposure**  
Do not let product enter drains.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance &amp; Form (crystalline)</td>
<td>Color (yellow)</td>
</tr>
<tr>
<td>b) Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>c) Odor threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: 84 - 86 °C (183 - 187 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point</td>
<td>297 °C 567 °F - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>150 °C (302 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or</td>
<td>No data available</td>
</tr>
<tr>
<td>explosive limits</td>
<td></td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>No data available</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>No data available</td>
</tr>
</tbody>
</table>
m) Density  1.368 g/cm³ at 25 °C (77 °F) - lit.
   Relative density  No data available
n) Water solubility  No data available
o) Partition coefficient: n-octanol/water  No data available
p) Autoignition temperature  No data available
q) Decomposition temperature  No data available
r) Viscosity  No data available
s) Explosive properties  No data available
t) Oxidizing properties  none

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.
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.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Oxidizing agents
Reducing agents
Strong bases

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5
SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
Acute toxicity estimate Oral - 5.01 mg/kg
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute toxicity estimate Inhalation - 4 h - 0.0501 mg/l - dust/mist
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute toxicity estimate Dermal - 5 mg/kg
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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
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.
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard
No data available

11.2 Additional Information

RTECS: CZ7350000
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., Cough, Shortness of breath, Headache, Nausea, Vomiting
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
SECTION 12: Ecological information

12.1 Toxicity
No data available

12.2 Persistence and degradability
Biodegradability Result: According to the results of tests of biodegradability this product is not readily biodegradable.

12.3 Bioaccumulative potential
No data available

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 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Product
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

DOT (US)
UN number: 3443 Class: 6.1 Packing group: II
Proper shipping name: Dinitrobenzenes, solid
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 3443 Class: 6.1 Packing group: II
EMS-No: F-A, S-A
Proper shipping name: DINITROBENZENES, SOLID

Sigma-Aldrich - 45966
Marine pollutant : yes

IATA
UN number: 3443    Class: 6.1    Packing group: II
Proper shipping name: Dinitrobenzenes, solid

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Dinitrobenzene</td>
<td>99-65-0</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

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

Massachusetts Right To Know Components
m-Dinitrobenzene

Pennsylvania Right To Know Components
m-Dinitrobenzene

California Prop. 65 Components
m-Dinitrobenzene

, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.m-Dinitrobenzene

SECTION 16: Other information

Further information
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.

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