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

1.1 Product identifiers

Product name : 1,3,5-Trinitrobenzene

Product Number : 442237
Brand : Supelco
Index-No. : 609-005-00-8
CAS-No. : 99-35-4

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)

Explosives (Division 1.1), H201
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

Supelco - 442237
Pictogram

Signal Word Danger

Hazard statement(s)
H201 Explosive; mass explosion hazard.
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)
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P230 Keep wetted with water.
P240 Ground/bond container and receiving equipment.
P250 Do not subject to grinding/ shock/ friction.
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/ eye protection/ face protection.
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.
P370 + P380 In case of fire: Evacuate area.
P372 Explosion risk in case of fire.
P373 DO NOT fight fire when fire reaches explosives.
P391 Collect spillage.
P401 Store in accordance with local regulations.
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

Formula : C₆H₃N₃O₆
Molecular weight: 213.10 g/mol
CAS-No.: 99-35-4
EC-No.: 202-752-7
Index-No.: 609-005-00-8

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3,5-Trinitrobenzene</td>
<td>Expl. 1.1; Acute Tox. 2; Acute Tox. 1; STOT RE 2; Aquatic Acute 1; Aquatic Chronic 1; H201, H300, H330, H310, H373, H400, H410 M-Factor - Aquatic Acute: 10</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

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

Supelco - 442237

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
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.
In the event of decomposition: danger of explosion!
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.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition.
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
Keep locked up or in an area accessible only to qualified or authorized persons. Keep separate or only together with other explosive substances, keep away from sources of ignition and heat. Observe national regulations.

Storage class
Storage class (TRGS 510): 1: Explosive 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
Contains no substances with occupational exposure limit values.

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 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 EC 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**
Flame retardant antistatic 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. 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.

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

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**SECTION 9: Physical and chemical properties**

9.1 Information on basic physical and chemical properties

- **a)** Appearance
  - Form: solid
- **b)** Odor
  - No data available
- **c)** Odor Threshold
  - No data available
- **d)** pH
  - No data available
- **e)** Melting point/freezing point
  - No data available
- **f)** Initial boiling point and boiling range
  - No data available
- **g)** Flash point
  - No data available
- **h)** Evaporation rate
  - No data available
- **i)** Flammability (solid, gas)
  - No data available
- **j)** Upper/lower flammability or explosive limits
  - No data available
- **k)** Vapor pressure
  - No data available
- **l)** Vapor density
  - No data available
- **m)** Density
  - No data available
- **n)** Relative density
  - No data available
n) Water solubility  No data available
o) Partition coefficient:  
n-octanol/water  log Pow: 0.243
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
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
No data available

10.4 Conditions to avoid
no information available

10.5 Incompatible materials
Strong oxidizing agents

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 - 5.1 mg/kg
(Expert judgment)
LC50 Inhalation - 4 h - 0.051 mg/l - dust/mist

Acute toxicity estimate Dermal - 5.1 mg/kg
(Expert judgment)
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
May cause damage to organs through prolonged or repeated exposure.

Remarks: No data available

Aspiration hazard
No data available

11.2 Additional Information
RTECS: DC3850000
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., Nausea, Dizziness, Headache, Lethargy., Cough, chest pain, Difficulty in breathing

SECTION 12: Ecological information

12.1 Toxicity
Toxicity to fish LC50 - Oncorhynchus mykiss (rainbow trout) - 0.52 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h

12.2 Persistence and degradability
No data available
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. Explosive materials: transport and disposal only in sufficiently desensitised condition!

SECTION 14: Transport information

DOT (US)
UN number: 0000    Class: NON
Proper shipping name: “unable to ship at this time”
Reportable Quantity (RQ): 10 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 0000    Class: NON
EMS-No: F-A, S-M
Not permitted for transport

IATA
UN number: 0000    Class: NON
Proper shipping name: “unable to ship at this time”
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

Further information
Unable to ship at this time, further testing needed.
SECTION 15: Regulatory information

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

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
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

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Pennsylvania Right To Know Components

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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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