SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: \( N,N'\)-Di-\( \text{tert} \)-butylcarbodiimide

Product Number: 235563
Brand: Aldrich
CAS-No.: 691-24-7

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)

- Flammable liquids (Category 3), H226
- 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: Warning

Aldrich - 235563
Hazard statement(s)
H226  Flammable liquid and vapor.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H335  May cause respiratory irritation.

Precautionary statement(s)
P210  Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233  Keep container tightly closed.
P240  Ground/bond container and receiving equipment.
P241  Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242  Use only non-sparking tools.
P243  Take precautionary measures against static discharge.
P261  Avoid breathing mist or vapors.
P264  Wash skin thoroughly after handling.
P271  Use only outdoors or in a well-ventilated area.
P280  Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353  IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312  IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338  IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313  If skin irritation occurs: Get medical advice/ attention.
P337 + P313  If eye irritation persists: Get medical advice/ attention.
P362  Take off contaminated clothing and wash before reuse.
P370 + P378  In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233  Store in a well-ventilated place. Keep container tightly closed.
P403 + P235  Store in a well-ventilated place. Keep cool.
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: C₉H₁₈N₂
Molecular weight: 154.25 g/mol
CAS-No.: 691-24-7
EC-No.: 211-719-6

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Di-tert-butylcarbodiimide</td>
<td>Flam. Liq. 3; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H226, H315, H319, H335</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Aldrich - 235563
SECTION 4: First aid measures

4.1 Description of 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.

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

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
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 at elevated temperatures.
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**  
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**  
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

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**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**

**Advice on protection against fire and explosion**  
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**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 container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store under inert gas. Moisture sensitive. Exposure to moisture.

**Storage class**  
Storage class (TRGS 510): 3: Flammable liquids

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**
required

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter type ABEK
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 vapours/aerosols 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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: clear, liquid
   Color: colorless

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
   48 - 50 °C 118 - 122 °F at 16 hPa

and boiling range

g) Flash point
   35 °C (95 °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) Vapor pressure  No data available
l) Vapor density  No data available
m) Density  0.8 g/mL at 25 °C (77 °F)
   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  No data available

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

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
Heating.

10.5 Incompatible materials
Strong acids

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**
- Oral: No data available
- Inhalation: No data available
- Dermal: No data available
- No data available

**Skin corrosion/irritation**
Remarks: No data available

**Serious eye damage/eye irritation**
Remarks: 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**
- Inhalation: May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

11.2 Additional Information
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
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.

SECTION 14: Transport information

DOT (US)
UN number: 1993  Class: 3  Packing group: III
Proper shipping name: Flammable liquids, n.o.s. (Di-tert-butylcarbodiimide)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 1993  Class: 3  Packing group: III  EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (Di-tert-butylcarbodiimide)

IATA
UN number: 1993  Class: 3  Packing group: III
Proper shipping name: Flammable liquid, n.o.s. (Di-tert-butylcarbodiimide)

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

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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