

## SAFETY DATA SHEET

Version 5.2  
Revision Date 10/14/2016  
Print Date 09/08/2019

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 1-tert-Butyl-3,4,5-trimethyl-2,6-dinitrobenzene

Product Number : S359165

Brand : Aldrich

CAS-No. : 145-39-1

## 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 # : +1-703-527-3887 (CHEMTREC)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

## 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

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

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3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Formula :  $C_{13}H_{18}N_2O_4$

Molecular weight : 266.3 g/mol

CAS-No. : 145-39-1

EC-No. : 205-651-6

No components need to be disclosed according to the applicable regulations.

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4. FIRST AID MEASURES

## 4.1 Description of first aid measures

**If inhaled**

If breathed in, move person into fresh air. If not breathing give artificial respiration

**In case of skin contact**

Wash off with soap and plenty of water.

**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.

**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

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**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

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Avoid dust formation.

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**

Sweep up and shovel. Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Provide appropriate exhaust ventilation at places where dust is formed. 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.

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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**8. EXPOSURE CONTROLS/PERSONAL PROTECTION****8.1 Control parameters****Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

**8.2 Exposure controls****Appropriate engineering controls**

General industrial hygiene practice.

## Personal protective equipment

### Eye/face protection

Safety glasses

### Skin protection

For prolonged or repeated contact use protective gloves.

### Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 133 - 136 °C (271 - 277 °F)
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) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	No data available
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

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## 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, Strong bases

## 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)  
In the event of fire: see section 5

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# 11. TOXICOLOGICAL INFORMATION

## 11.1 Information on toxicological effects

### Acute toxicity

LD50 Oral - Rat - > 6,000 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - > 5,000 mg/kg

No data available

### Skin corrosion/irritation

### Serious eye damage/eye irritation

Eyes - Rabbit

### Respiratory or skin sensitisation

### Germ cell mutagenicity

### 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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

No data available

### Specific target organ toxicity - single exposure

### Specific target organ toxicity - repeated exposure

### Aspiration hazard

### Additional Information

RTECS: CZ7220000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

### 12.2 Persistence and degradability

### 12.3 Bioaccumulative potential

### 12.4 Mobility in soil

### 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

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Observe all federal, state, and local environmental regulations.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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## 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

No SARA Hazards

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1-tert-Butyl-3,4,5-trimethyl-2,6-dinitrobenzene	145-39-1	2009-07-17

### New Jersey Right To Know Components

	CAS-No.	Revision Date
1-tert-Butyl-3,4,5-trimethyl-2,6-dinitrobenzene	145-39-1	2009-07-17

### 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.

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## 16. OTHER INFORMATION

### HMIS Rating

Health hazard:	0
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

### NFPA Rating

Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	0

### Further information

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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](http://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

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