SAFETY DATA SHEET
N-tert-Butylbenzenesulfinimidoyl chloride

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

1.1. Product identifier
Product name N-tert-Butylbenzenesulfinimidoyl chloride
Product number FB61005
Synonyms; trade names N-tert-Butylphenylsulfinimidoyl Chloride
CAS number 49591-20-0

1.2. Relevant identified uses of the substance or mixture and uses advised against
Identified uses Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet
Supplier Carbosynth Ltd
8&9 Old Station Business Park
Compton
Berkshire
RG20 6NE
UK
+44 1635 578444
+44 1635 579444
info@carbosynth.com

1.4. Emergency telephone number
Emergency telephone +44 7887 998634

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture
Classification (EC 1272/2008)
Health hazards Skin Corr. 1C - H314 Eye Dam. 1 - H318
Environmental hazards Not Classified

2.2. Label elements
Pictogram
Signal word Danger
Hazard statements H290 May be corrosive to metals.
H314 Causes severe skin burns and eye damage.
N-tert-Butylbenzenesulfinimidoyl chloride

Precautionary statements
P264 Wash contaminated skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name N-tert-Butylbenzenesulfinimidoyl chloride
CAS number 49591-20-0
Chemical formula C₆H₄ClN₃S

SECTION 4: First aid measures

4.1. Description of first aid measures
General information Get medical advice/attention if you feel unwell.
Inhalation Remove person to fresh air and keep comfortable for breathing. If breathing stops, provide artificial respiration. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention if symptoms are severe or persist.
Ingestion Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed
General information See Section 11 for additional information on health hazards.

4.3. Indication of any immediate medical attention and special treatment needed
Notes for the doctor Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media
Suitable extinguishing media Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

5.2. Special hazards arising from the substance or mixture
Specific hazards None known.
Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen. Oxides of sulphur. Hydrogen chloride (HCl).

5.3. Advice for firefighters
N-tert-Butylbenzenesulfinimidoyl chloride

Special protective equipment for firefighters
Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions
Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust and vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage.

6.2. Environmental precautions

Environmental precautions
Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up
Wear protective clothing as described in Section 8 of this safety data sheet. Collect powder using special dust vacuum cleaner with particle filter or carefully sweep into suitable waste disposal containers and seal securely. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections
For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions
Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid generation and spreading of dust. Avoid contact with skin and eyes. Avoid inhalation of dust and vapours.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions
Keep container tightly closed. Store away from incompatible materials (see Section 10). Keep away from heat. Protect from moisture. Store contents under inert gas. Store at temperatures not exceeding -20°C.

7.3. Specific end use(s)

Specific end use(s)
The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits
No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls
Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection
Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.
N-tert-Butylbenzenesulfinimidoyl chloride

Hand protection
Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

Other skin and body protection
Wear appropriate clothing to prevent repeated or prolonged skin contact.

Respiratory protection
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Particulate filters should comply with European Standard EN143. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

Environmental exposure controls
Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Solid</td>
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<tr>
<td>Colour</td>
<td>Yellow to Red</td>
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<tr>
<td>Odour</td>
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<td>Odour threshold</td>
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<td>pH</td>
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<td>Melting point</td>
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<tr>
<td>Initial boiling point and range</td>
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<td>Flash point</td>
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<tr>
<td>Evaporation rate</td>
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<tr>
<td>Flammability (solid, gas)</td>
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<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>No data available</td>
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<tr>
<td>Vapour pressure</td>
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<tr>
<td>Vapour density</td>
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</tr>
<tr>
<td>Relative density</td>
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</tr>
<tr>
<td>Solubility(ies)</td>
<td>Miscible with the following materials: Toluene</td>
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<tr>
<td>Partition coefficient</td>
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<tr>
<td>Auto-ignition temperature</td>
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<tr>
<td>Decomposition Temperature</td>
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<tr>
<td>Viscosity</td>
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<tr>
<td>Explosive properties</td>
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</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2. Other information

Molecular weight
215.74

SECTION 10: Stability and reactivity
N-tert-Butylbenzenesulfinimidoyl chloride

10.1. Reactivity
Reactivity
No data available.

10.2. Chemical stability
Stability
Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions
Possibility of hazardous reactions
No data available.

10.4. Conditions to avoid
Conditions to avoid
Moisture.

10.5. Incompatible materials
Materials to avoid
Oxidising agents.

10.6. Hazardous decomposition products
Hazardous decomposition products

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral
Notes (oral LD₅₀)
Based on available data the classification criteria are not met.

Acute toxicity - dermal
Notes (dermal LD₅₀)
Based on available data the classification criteria are not met.

Acute toxicity - inhalation
Notes (inhalation LC₅₀)
Based on available data the classification criteria are not met.

Skin corrosion/irritation
Animal data
Skin Corr. 1C - H314 Causes severe burns.

Serious eye damage/irritation
Eye Dam. 1 - H318 Corrosive to skin. Corrosivity to eyes is assumed.

Respiratory sensitisation
Based on available data the classification criteria are not met.

Skin sensitisation
Based on available data the classification criteria are not met.

Germ cell mutagenicity
Based on available data the classification criteria are not met.

Carcinogenicity
Based on available data the classification criteria are not met.

IARC carcinogenicity
None of the ingredients are listed or exempt.

Reproductive toxicity
Based on available data the classification criteria are not met.

Reproductive toxicity - fertility
Based on available data the classification criteria are not met.

Reproductive toxicity - development
Based on available data the classification criteria are not met.
N-tert-Butylbenzenesulfinimidoyl chloride

Specific target organ toxicity - single exposure
STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure
STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard
Aspiration hazard Not relevant. Solid.

General information Dust may irritate the eyes and the respiratory system. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation Corrosive to the respiratory tract. Symptoms following overexposure may include the following: Severe irritation of nose and throat.

Ingestion May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.

Skin contact Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.

Eye contact Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs No specific target organs known.

SECTION 12: Ecological Information

Ecotoxicity Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity Toxicity Based on available data the classification criteria are not met.

12.2. Persistence and degradability Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No data available.

12.4. Mobility in soil Mobility No data available.

12.5. Results of PBT and vPvB assessment Results of PBT and vPvB assessment No data available.

12.6. Other adverse effects Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods
N-tert-Butylbenzenesulfinimidoyl chloride

**General information**
Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

**Disposal methods**
Mix or dissolve the material in a combustible solvent and burn in chemical incinerator equipped with an afterburner and scrubber.

### SECTION 14: Transport information

14.1. **UN number**
- UN No. (ADR/RID) 3261
- UN No. (IMDG) 3261
- UN No. (ICAO) 3261
- UN No. (ADN) 3261

14.2. **UN proper shipping name**
- Proper shipping name (ADR/RID) CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-tert-Butylbenzenesulfinimidoyl chloride)
- Proper shipping name (IMDG) CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-tert-Butylbenzenesulfinimidoyl chloride)
- Proper shipping name (ICAO) CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-tert-Butylbenzenesulfinimidoyl chloride)
- Proper shipping name (ADN) CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-tert-Butylbenzenesulfinimidoyl chloride)

14.3. **Transport hazard class(es)**
- ADR/RID class 8
- ADR/RID classification code C4
- ADR/RID label 8
- IMDG class 8
- ICAO class/division 8
- ADN class 8

14.4. **Packing group**
- ADR/RID packing group III
- IMDG packing group III
- ADN packing group III
- ICAO packing group III

14.5. **Environmental hazards**
- Environmentally hazardous substance/marine pollutant No.

14.6. **Special precautions for user**
N-tert-Butylbenzenesulfinimidoyl chloride

IMDG Code segregation group 1. Acids
EmS F-A, S-B
ADR transport category 3
Emergency Action Code 2X
Hazard Identification Number (ADR/RID) 80
Tunnel restriction code (E)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations
Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.

EU legislation

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet
ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
IATA: International Air Transport Association.
IMDG: International Maritime Dangerous Goods.
CAS: Chemical Abstracts Service.
ATE: Acute Toxicity Estimate.
LC₅₀: Lethal Concentration to 50 % of a test population.
LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).
EC₅₀: 50% of maximal Effective Concentration.
PBT: Persistent, Bioaccumulative and Toxic substance.
vPvB: Very Persistent and Very Bioaccumulative.

Training advice
Only trained personnel should use this material.

Revision date 01/02/2018
Revision 1
SDS number 144926
**N-tert-Butylbenzenesulfinimidoyl chloride**

<table>
<thead>
<tr>
<th>Hazard statements in full</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>H290</td>
<td>May be corrosive to metals.</td>
</tr>
<tr>
<td>H314</td>
<td>Causes severe skin burns and eye damage.</td>
</tr>
<tr>
<td>H318</td>
<td>Causes serious eye damage.</td>
</tr>
</tbody>
</table>

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.