SAFETY DATA SHEET
4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester

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

#### 1.1. Product identifier
- **Product name**: 4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester
- **Product number**: FT05936
- **CAS number**: 97600-39-0

#### 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)**
  - **Physical hazards**: Not Classified
  - **Health hazards**: Not Classified
  - **Environmental hazards**: Not Classified

#### 2.2. Label elements
- **Hazard statements**: NC Not Classified

#### 2.3. Other hazards
- **No data available.**

### SECTION 3: Composition/information on ingredients

#### 3.1. Substances
- **Product name**: 4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester
- **CAS number**: 97600-39-0
- **Chemical formula**: C₆₀H₈₀O₁₂
4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester

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 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.

5.3. Advice for firefighters

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
4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester

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 in a cool and well-ventilated place. Store away from incompatible materials (see Section 10). Protect from light. Store at room temperature.

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.

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 filter, type P1. 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
4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester

9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Solid</td>
</tr>
<tr>
<td>Colour</td>
<td>White to Yellow</td>
</tr>
<tr>
<td>Odour</td>
<td>No data available</td>
</tr>
<tr>
<td>Odour threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting point</td>
<td>155°C</td>
</tr>
<tr>
<td>Initial boiling point and range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapour density</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Solubility(ies)</td>
<td>No data available</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>No data available</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition Temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2. Other information

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>993.27</td>
</tr>
</tbody>
</table>

SECTION 10: Stability and reactivity

10.1. Reactivity

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactivity</td>
<td>No data available</td>
</tr>
</tbody>
</table>

10.2. Chemical stability

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability</td>
<td>Stable under the prescribed storage conditions.</td>
</tr>
</tbody>
</table>

10.3. Possibility of hazardous reactions

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Possibility of hazardous reactions</td>
<td>No data available.</td>
</tr>
</tbody>
</table>

10.4. Conditions to avoid

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conditions to avoid</td>
<td>No data available.</td>
</tr>
</tbody>
</table>

10.5. Incompatible materials

<table>
<thead>
<tr>
<th>Property</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Materials to avoid</td>
<td>Strong oxidising agents.</td>
</tr>
</tbody>
</table>
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10.6. Hazardous decomposition products

| Hazardous decomposition products | Oxides of carbon. |

SECTION 11: Toxicological information

11.1. Information on toxicological effects

<table>
<thead>
<tr>
<th>Toxicological effects</th>
<th>Not regarded as a health hazard under current legislation.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute toxicity - oral</td>
<td>Notes (oral LD₅₀) Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Acute toxicity - dermal</td>
<td>Notes (dermal LD₅₀) Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Acute toxicity - inhalation</td>
<td>Notes (Inhalation LC₅₀) Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Skin corrosion/irritation</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Animal data</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Serious eye damage/irritation</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Respiratory sensitisation</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Skin sensitisation</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Germ cell mutagenicity</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>IARC carcinogenicity</td>
<td>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.</td>
</tr>
<tr>
<td>Reproductive toxicity</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Reproductive toxicity - fertility</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Reproductive toxicity - development</td>
<td>Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td>Specific target organ toxicity - single exposure</td>
<td>STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.</td>
</tr>
<tr>
<td>Specific target organ toxicity - repeated exposure</td>
<td>STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.</td>
</tr>
<tr>
<td>Aspiration hazard</td>
<td>Not relevant. Solid.</td>
</tr>
<tr>
<td>General information</td>
<td>No specific health hazards known. 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.</td>
</tr>
</tbody>
</table>
**4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester**

<table>
<thead>
<tr>
<th>Route of exposure</th>
<th>Inhalation</th>
<th>Ingestion</th>
<th>Skin contact</th>
<th>Eye contact</th>
<th>Route of exposure</th>
<th>Target organs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dust may irritate the respiratory system. Frequent inhalation of dust over a long period of time increases the risk of developing lung diseases.</td>
<td>No specific symptoms known. May cause discomfort if swallowed.</td>
<td>Prolonged contact may cause dryness of the skin.</td>
<td>Dust may cause slight irritation.</td>
<td>Ingestion Inhalation Skin and/or eye contact</td>
<td>No specific target organs known.</td>
</tr>
</tbody>
</table>
**4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester**

### 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**
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.

### SECTION 14: Transport information

**General**
The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).

**14.1. UN number**
Not applicable.

**14.2. UN proper shipping name**
Not applicable.

**14.3. Transport hazard class(es)**
No transport warning sign required.

**14.4. Packing group**
Not applicable.

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

**14.6. Special precautions for user**
4-tert-Butylcalix[4]arene-tetraacetic acid tetraethyl ester

Not applicable.

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

Transport in bulk according to
Annex II of MARPOL 73/78
and the IBC Code

Not applicable.

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
29/10/2018

Revision
1

SDS number
144926

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