SAFETY DATA SHEET
1,1,3,3-Tetramethylbutyl isocyanide


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

1.1. Product identifier

Product name 1,1,3,3-Tetramethylbutyl isocyanide
Product number FT02696
Synonyms; trade names tert-Octyl isocyanide, Walborsky’s reagent
CAS number 14542-93-9
EC number 238-577-8

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 Flam. Liq. 3 - H226
Health hazards Acute Tox. 4 - H302 Acute Tox. 4 - H312 Acute Tox. 4 - H332
Environmental hazards Not Classified

2.2. Label elements

EC number 238-577-8

Pictogram

Signal word Warning
1,1,3,3-Tetramethylbutyl isocyanide

Hazard statements
H226 Flammable liquid and vapour.
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.

Precautionary statements
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302+P352 IF ON SKIN: Wash with plenty of water.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name 1,1,3,3-Tetramethylbutyl isocyanide
CAS number 14542-93-9
EC number 238-577-8
Chemical formula C₉H₁₇N

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. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. 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.
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Hazardous combustion products
Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen.

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 vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage. Eliminate all sources of ignition.

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. Absorb spillage with sand or other inert absorbent. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Provide adequate ventilation. 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 contact with skin and eyes. Do not breathe vapours. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

7.2. Conditions for safe storage, including any incompatibilities
Storage precautions
Keep container tightly closed. Store away from incompatible materials (see Section 10). Keep containers upright. Store contents under inert gas. Store at temperatures between 2°C and 8°C.

Storage class
Flammable liquid storage.

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
1,1,3,3-Tetramethylbutyl isocyanide

**Appropriate engineering controls**
Provide adequate ventilation.

**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. Gas and combination filter cartridges should comply with European Standard EN14387. 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>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Liquid.</td>
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<tr>
<td>Colour</td>
<td>Colourless. to Yellow.</td>
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<tr>
<td>Odour</td>
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<tr>
<td>Odour threshold</td>
<td>No data available.</td>
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<tr>
<td>pH</td>
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<tr>
<td>Melting point</td>
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<tr>
<td>Initial boiling point and range</td>
<td>55 to 57°C @ 15 hPa</td>
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<tr>
<td>Flash point</td>
<td>52°C Closed cup.</td>
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<tr>
<td>Evaporation rate</td>
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<td>Flammability (solid, gas)</td>
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<tr>
<td>Upper/lower flammability or</td>
<td>No data available.</td>
</tr>
<tr>
<td>explosive limits</td>
<td></td>
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<td>Vapour pressure</td>
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<tr>
<td>Vapour density</td>
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<tr>
<td>Relative density</td>
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<tr>
<td>Solubility(ies)</td>
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<td>Partition coefficient</td>
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<td>Auto-ignition temperature</td>
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<tr>
<td>Decomposition Temperature</td>
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</tr>
<tr>
<td>Viscosity</td>
<td>No data available.</td>
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</table>
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**Explosive properties**
No data available.

**Oxidising properties**
No data available.

**9.2. Other information**
Molecular weight 139.24

**SECTION 10: Stability and reactivity**

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  Keep away from heat, sparks and open flame.

10.5. Incompatible materials

Materials to avoid  Oxidising agents.

10.6. Hazardous decomposition products


**SECTION 11: Toxicological information**

11.1. Information on toxicological effects

**Acute toxicity - oral**

Notes (oral LD₅₀)  Acute Tox. 4 - H302 Harmful if swallowed.

ATE oral (mg/kg)  500.0

**Acute toxicity - dermal**

Notes (dermal LD₅₀)  Acute Tox. 4 - H312 Harmful in contact with skin.

ATE dermal (mg/kg)  1,100.0

**Acute toxicity - inhalation**

Notes (inhalation LC₅₀)  Acute Tox. 4 - H332 Harmful if inhaled.

ATE inhalation (vapours mg/l)  11.0

**Skin corrosion/irritation**

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

**Serious eye damage/irritation**

Serious eye damage/irritation  Based on available data the classification criteria are not met.

**Respiratory sensitisation**

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

**Skin sensitisation**

Skin sensitisation  Based on available data the classification criteria are not met.
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Germ cell mutagenicity
Genotoxicity - in vitro
Based on available data the classification criteria are not met.

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

IARC carcinogenicity
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.

Reproductive toxicity
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.

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
Based on available data the classification criteria are not met.

General information
The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation
A single exposure may cause the following adverse effects: Headache. Exhaustion and weakness.

Ingestion
May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.

Skin contact
May cause discomfort.

Eye contact
No specific symptoms known.

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
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**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.

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

### SECTION 14: Transport information

#### 14.1. UN number

- **UN No. (ADR/RID)**
  1993
- **UN No. (IMDG)**
  1993
- **UN No. (ICAO)**
  1993
- **UN No. (ADN)**
  1993

#### 14.2. UN proper shipping name

| Proper shipping name (ADR/RID) | FLAMMABLE LIQUID, N.O.S. (1,1,3,3-Tetramethylbutyl isocyanate) |
| Proper shipping name (IMDG)    | FLAMMABLE LIQUID, N.O.S. (1,1,3,3-Tetramethylbutyl isocyanate) |
| Proper shipping name (ICAO)    | FLAMMABLE LIQUID, N.O.S. (1,1,3,3-Tetramethylbutyl isocyanate) |
| Proper shipping name (ADN)     | FLAMMABLE LIQUID, N.O.S. (1,1,3,3-Tetramethylbutyl isocyanate) |

#### 14.3. Transport hazard class(es)

- **ADR/RID class**
  3
- **ADR/RID classification code**
  F1
- **ADR/RID label**
  3
- **IMDG class**
  3
- **ICAO class/division**
  3
- **ADN class**
  3

**Transport labels**

#### 14.4. Packing group

| ADR/RID packing group | III |
| IMDG packing group    | III |
1,1,3,3-Tetramethylbutyl isocyanide

ADN packing group  III
ICAO packing group  III

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

14.6. Special precautions for user
EmS  F-E, S-E
ADR transport category  3
Emergency Action Code  •3Y
Hazard Identification Number (ADR/RID)  30
Tunnel restriction code  (D/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.


15.2. Chemical safety assessment
No chemical safety assessment has been carried out.

Inventories
US - TSCA
Present.

SECTION 16: Other information

8/9
1,1,3,3-Tetramethylbutyl isocyanide

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
24/05/2017

Revision
1

SDS number
144929

Hazard statements in full
H226 Flammable liquid and vapour.
H302 Harmful if swallowed.
H312 Harmful in contact with skin.
H332 Harmful if inhaled.