SAFETY DATA SHEET
1-(Trifluoroacetyl)imidazole


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

1.1. Product identifier
Product name 1-(Trifluoroacetyl)imidazole
Product number FT60417
CAS number 1546-79-8
EC number 216-282-5

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 Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 STOT SE 3 - H335
Environmental hazards Not Classified

2.2. Label elements
EC number 216-282-5

Pictogram

Signal word Warning

Hazard statements H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
1-(Trifluoroacetyl)imidazole

Precautionary statements
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P264 Wash contaminated skin thoroughly after handling.
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.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313 If eye irritation persists: Get medical advice/ attention.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name 1-(Trifluoroacetyl)imidazole
CAS number 1546-79-8
EC number 216-282-5
Chemical formula C₅H₃F₃N₂O

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 a few small glasses of water or milk 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.
1-(Trifluoroacetyl)imidazole

**Hazardous combustion products**
Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen. Hydrogen fluoride (HF).

**5.3. Advice 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. Eliminate all sources of ignition. Keep unnecessary and unprotected personnel away from the spillage. Vapour from residual product may create a highly flammable or explosive atmosphere inside the container. Vapours may accumulate on the floor and in low-lying areas.

**6.2. 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. Eliminate all sources of ignition. For waste disposal, see Section 13.

**6.4. 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. Avoid inhalation of vapours and spray/mists. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge.

**7.2. Conditions for safe storage, including any incompatibilities**

**Storage precautions**
Keep container tightly closed. Store in a cool and well-ventilated place. Keep containers upright. Store away from incompatible materials (see Section 10). Store contents under inert gas. Handle under inert gas. Protect from moisture. Keep away from heat. Store at temperatures between 2°C and 8°C.

**7.3. 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**
1-(Trifluoroacetyl)imidazole

No exposure limits known for ingredient(s).

8.2. Exposure controls

**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.

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**SECTION 9: Physical and Chemical Properties**

**9.1. Information on basic physical and chemical properties**

- **Appearance**: Liquid.
- **Odour threshold**: No data available.
- **pH**: No data available.
- **Initial boiling point and range**: 45 to 46°C @ 19 hPa
- **Flash point**: 44°C Closed cup.
- **Evaporation rate**: No data available.
- **Flammability (solid, gas)**: No data available.
- **Upper/lower flammability or explosive limits**: No data available.
- **Vapour pressure**: No data available.
- **Vapour density**: No data available.
- **Relative density**: 1.442 g/cm³ @ 25°C
- **Solubility(ies)**: No data available.
- **Partition coefficient**: No data available.
- **Auto-ignition temperature**: No data available.
- **Decomposition Temperature**: No data available.
- **Viscosity**: No data available.
- **Explosive properties**: No data available.
1-(Trifluoroacetyl)imidazole

Oxidising properties
No data available.

9.2. Other information
Molecular weight 164.09

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 Heat, sparks, flames. Take precautionary measures against static discharges.

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) 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 Irritating.

Serious eye damage/irritation
Serious eye damage/irritation Causes serious eye irritation.

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.

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.
1-(Trifluoroacetyl)imidazole

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 STOT SE 3 - H335 May cause respiratory irritation.
Target organs Respiratory system, lungs

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: Irritation of nose, throat and airway. Difficulty in breathing. Coughing.

Ingestion
May cause irritation.

Skin contact
Redness. Irritating to skin.

Eye contact
Irritating to eyes.

Route of exposure
Ingestion Inhalation Skin and/or eye contact

Target organs Respiratory system, lungs

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 This substance is not classified as PBT or vPvB according to current EU criteria.

12.6. Other adverse effects
1-(Trifluoroacetyl)imidazole

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

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-(Trifluoroacetyl)imidazole) |
| Proper shipping name (IMDG) | FLAMMABLE LIQUID, N.O.S. (1-(Trifluoroacetyl)imidazole) |
| Proper shipping name (ICAO) | FLAMMABLE LIQUID, N.O.S. (1-(Trifluoroacetyl)imidazole) |
| Proper shipping name (ADN) | FLAMMABLE LIQUID, N.O.S. (1-(Trifluoroacetyl)imidazole) |

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 |
| ADN packing group | III |
| ICAO packing group | III |

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant
No.
1-((Trifluoroacetyl)imidazole)

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.

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: 13/10/2017

Revision: 1

SDS number: 144929
1-(Trifluoroacetyl)imidazole

Hazard statements in full

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

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.