

4-(TRIFLUOROMETHYL)BENZYL ISOCYANATE

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

### 1.1. Product identifier

Product name: 4-(TRIFLUOROMETHYL)BENZYL ISOCYANATE

**CAS number:** 102422-55-9 **Product code:** PC904664

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

# 1.3. Details of the supplier of the safety data sheet

Company name: Apollo Scientific Ltd

Units 3 & 4
Parkway
Denton
Manchester
M34 3SG
UK

**Tel:** 0161 337 9971 **Fax:** 0161 336 6932

Email: david.tideswell@apolloscientific.co.uk

# 1.4. Emergency telephone number

# Section 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification under CLP: Acute Tox. 3: H301+311+331

Most important adverse effects: Toxic if swallowed, in contact with skin or if inhaled.

### 2.2. Label elements

Label elements:

Hazard statements: H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.

Signal words: Danger

Hazard pictograms: GHS06: Skull and crossbones



Precautionary statements: P260: Do not breathe vapours.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

P301+310: IF SWALLOWED: Immediately call a POISON CENTER.

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### 2.3. Other hazards

**PBT:** This product is not identified as a PBT/vPvB substance.

## Section 3: Composition/information on ingredients

#### 3.1. Substances

Chemical identity: 4-(TRIFLUOROMETHYL)BENZYL ISOCYANATE

CAS number: 102422-55-9

## Section 4: First aid measures

# 4.1. Description of first aid measures

Skin contact: Remove all contaminated clothes and footwear immediately unless stuck to skin.

Drench the affected skin with running water for 10 minutes or longer if substance is still

on skin. Transfer to hospital if there are burns or symptoms of poisoning.

Eye contact: Bathe the eye with running water for 15 minutes. Transfer to hospital for specialist

examination.

Ingestion: Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water

to drink immediately. If unconscious, check for breathing and apply artificial respiration if necessary. If unconscious and breathing is OK, place in the recovery position. Transfer

to hospital as soon as possible.

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. If

conscious, ensure the casualty sits or lies down. If unconscious and breathing is OK, place in the recovery position. If unconscious, check for breathing and apply artificial respiration if necessary. If breathing becomes bubbly, have the casualty sit and provide

oxygen if available. Transfer to hospital as soon as possible.

## 4.2. Most important symptoms and effects, both acute and delayed

Skin contact: There may be redness or whiteness of the skin in the area of exposure. Irritation or pain

may occur at the site of contact. Absorption through the skin may be fatal.

**Eye contact:** There may be severe pain. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. There may be vomiting.

Convulsions may occur. There may be loss of consciousness.

Inhalation: There may be shortness of breath with a burning sensation in the throat. Absorption

through the lungs can occur causing symptoms similar to those of ingestion.

Convulsions may occur. There may be loss of consciousness.

## 4.3. Indication of any immediate medical attention and special treatment needed

## Section 5: Fire-fighting measures

# 5.1. Extinguishing media

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the

surrounding fire should be used. Use water spray to cool containers.

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### 5.2. Special hazards arising from the substance or mixture

**Exposure hazards:** Toxic. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen

oxides (NOx). Hydrogen fluoride (HF). Hydrogen cyanide (HCN).

### 5.3. Advice for fire-fighters

Advice for fire-fighters: Wear self-contained breathing apparatus. Wear protective clothing to prevent contact

with skin and eyes.

### Section 6: Accidental release measures

# 6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions: Notify the police and fire brigade immediately. If outside do not approach from

downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel. Do not attempt to take action without suitable protective clothing - see section 8 of SDS. Turn

leaking containers leak-side up to prevent the escape of liquid.

### 6.2. Environmental precautions

Environmental precautions: Do not discharge into drains or rivers. Contain the spillage using bunding.

# 6.3. Methods and material for containment and cleaning up

Clean-up procedures: Clean-up should be dealt with only by qualified personnel familiar with the specific

substance. Absorb into dry earth or sand. Transfer to a closable, labelled salvage

container for disposal by an appropriate method.

### 6.4. Reference to other sections

# Section 7: Handling and storage

# 7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Ensure there is exhaust ventilation of the area.

Avoid the formation or spread of mists in the air. Only use in fume hood.

# 7.2. Conditions for safe storage, including any incompatibilities

**Storage conditions:** Store in a cool, well ventilated area. Keep container tightly closed. Recommended

storage temp 2-8 °C. Air sensitive. Store under Argon.

Suitable packaging: Must only be kept in original packaging.

## 7.3. Specific end use(s)

Specific end use(s): No data available.

### Section 8: Exposure controls/personal protection

# 8.1. Control parameters

Workplace exposure limits: No data available.

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### **DNEL/PNEC Values**

**DNEL / PNEC** No data available.

# 8.2. Exposure controls

Engineering measures: Ensure there is exhaust ventilation of the area.

**Respiratory protection:** Self-contained breathing apparatus must be available in case of emergency.

Hand protection: Impermeable gloves.

**Eye protection:** Safety glasses with side-shields. Ensure eye bath is to hand.

**Skin protection:** Impermeable protective clothing.

## Section 9: Physical and chemical properties

## 9.1. Information on basic physical and chemical properties

State: Liquid

Evaporation rate: No data available.

Oxidising: No data available.

Solubility in water: No data available.

Viscosity: No data available.

Boiling point/range ℃: No data available. Melting point/range ℃: No data available.

Flammability limits %: lower: No data available. upper: No data available.

Flash point °C: No data available. Part.coeff. n-octanol/water: No data available.

Autoflammability °C: No data available. Vapour pressure: No data available.

Relative density: No data available. pH: No data available.

VOC g/I: No data available.

#### 9.2. Other information

Other information: No data available.

# Section 10: Stability and reactivity

## 10.1. Reactivity

Reactivity: Stable under recommended transport or storage conditions.

# 10.2. Chemical stability

Chemical stability: Stable under normal conditions.

# 10.3. Possibility of hazardous reactions

Hazardous reactions: Hazardous reactions will not occur under normal transport or storage conditions.

### 10.4. Conditions to avoid

Conditions to avoid: Heat. Hot surfaces. Flames. Air.

### 10.5. Incompatible materials

Materials to avoid: Strong oxidising agents. Strong acids.

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# 10.6. Hazardous decomposition products

Haz. decomp. products: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides

(NOx). Hydrogen fluoride (HF). Hydrogen cyanide (HCN).

# **Section 11: Toxicological information**

# 11.1. Information on toxicological effects

### Relevant hazards for product:

Hazard	Route	Basis
Acute toxicity (ac. tox. 3)	INH DRM ING	Hazardous: calculated

### Symptoms / routes of exposure

Skin contact: There may be redness or whiteness of the skin in the area of exposure. Irritation or pain

may occur at the site of contact. Absorption through the skin may be fatal.

**Eye contact:** There may be severe pain. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. There may be vomiting.

Convulsions may occur. There may be loss of consciousness.

Inhalation: There may be shortness of breath with a burning sensation in the throat. Absorption

through the lungs can occur causing symptoms similar to those of ingestion.

Convulsions may occur. There may be loss of consciousness.

## Section 12: Ecological information

# 12.1. Toxicity

Ecotoxicity values: No data available.

# 12.2. Persistence and degradability

Persistence and degradability: No data available.

#### 12.3. Bioaccumulative potential

Bioaccumulative potential: No data available.

## 12.4. Mobility in soil

Mobility: No data available.

# 12.5. Results of PBT and vPvB assessment

PBT identification: This product is not identified as a PBT/vPvB substance.

### 12.6. Other adverse effects

Other adverse effects: No data available.

# Section 13: Disposal considerations

# 13.1. Waste treatment methods

Disposal operations: Transfer to a suitable container and arrange for collection by specialised disposal

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company. MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL,

STATE AND FEDERAL REGULATIONS

Disposal of packaging: Dispose of as special waste in compliance with local and national regulations Observe

all federal, state and local environmental regulations.

NB: The user's attention is drawn to the possible existence of regional or national

regulations regarding disposal.

# **Section 14: Transport information**

### 14.1. UN number

UN number: UN2206

# 14.2. UN proper shipping name

Shipping name: ISOCYANATES, TOXIC, N.O.S.

## 14.3. Transport hazard class(es)

Transport class: 6.1

### 14.4. Packing group

Packing group: III

## 14.5. Environmental hazards

Environmentally hazardous: No Marine pollutant: No

# 14.6. Special precautions for user

Tunnel code: E

Transport category: 2

## **Section 15: Regulatory information**

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

Specific regulations: Not applicable.

### 15.2. Chemical Safety Assessment

Chemical safety assessment: A chemical safety assessment has not been carried out for the substance or the mixture

by the supplier.

# **Section 16: Other information**

### Other information

**Other information:** This safety data sheet is prepared in accordance with Commission Regulation (EU) No 2015/830.

\* Data predicted using computational software. The OECD QSAR-Toolbox for grouping chemicals into categories. Developed by LMC bulgaria.

http://echa.europa.eu/support/oecd-qsar-toolbox

~ Data predicted using computational software ACD/ToxSuite v 2.95.1 Copyright 1994-

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2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry Development, Inc (ACD/Labs). http://www.acdlabs.com/products/pc\_admet/tox/tox/

Phrases used in s.2 and s.3: H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.

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