

## SAFETY DATA SHEET

Version 8.7  
Revision Date 09/07/2024  
Print Date 09/08/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Azido-4-fluorobenzene solution

Product Number : 779253

Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - repeated exposure (Category 1), H372

For the full text of the H-Statements mentioned in this Section, see Section 16.

Aldrich - 779253

Page 1 of 13

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225

Highly flammable liquid and vapor.

H315

Causes skin irritation.

H319

Causes serious eye irritation.

H372

Causes damage to organs through prolonged or repeated exposure.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use only non-sparking tools.

P243

Take precautionary measures against static discharge.

P260

Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P280

Wear protective gloves/ eye protection/ face protection.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P314

Get medical advice/ attention if you feel unwell.

P332 + P313

If skin irritation occurs: Get medical advice/ attention.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P403 + P235

Store in a well-ventilated place. Keep cool.

P501

Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.2 Mixtures

Synonyms : 4-Fluorophenyl azide solution

Formula :  $C_6H_4FN_3$

Molecular weight : 137.11 g/mol

| Component | Classification | Concentration |
|-----------|----------------|---------------|
|-----------|----------------|---------------|

| tert-butyl methyl ether |                       |  |                  |
|-------------------------|-----------------------|--|------------------|
| CAS-No.                 | 1634-04-4             | Flam. Liq. 2; Skin Irrit. 2;<br>H225, H315   | >= 90 - <= 100 % |
| EC-No.                  | 216-653-1             |  |                  |
| Index-No.               | 603-181-00-X          |  |                  |
| Registration number     | 01-2119452786-27-XXXX |  |                  |
|                         |                       |  |                  |
| 1-Azido-4-fluorobenzene |                       |  |                  |
| CAS-No.                 | 3296-02-4             | Self-react. B; Skin Irrit. 2;<br>Eye Irrit. 2A; STOT SE 3;<br>STOT RE 1; H241, H315,<br>H319, H335, H372 | >= 10 - < 20 %   |

For the full text of the H-Statements mentioned in this Section, see Section 16.

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

---

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Foam Carbon dioxide (CO2) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen fluoride

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

## **5.3 Advice for firefighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

## **5.4 Further information**

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains. Risk of explosion.

### **6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### **6.4 Reference to other sections**

For disposal see section 13.

---

## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

### Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage stability** Recommended storage temperature

-20 °C

Light sensitive. Over time, pressure may increase causing containers to burst

### Storage class

Storage class (TRGS 510): 3: Flammable liquids

## 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

| Component               | CAS-No.   | Value  | Control parameters              | Basis   |
|-------------------------|-----------|--|---------------------------------|---|
| tert-butyl methyl ether | 1634-04-4 | TWA  | 50 ppm                          | USA. ACGIH Threshold Limit Values (TLV)   |
|                         | Remarks   | Confirmed animal carcinogen with unknown relevance to humans |                                 |   |
|                         |           | PEL  | 40 ppm<br>144 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

### 8.2 Exposure controls

#### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 120 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **Body Protection**

Flame retardant antistatic protective clothing.

### **Respiratory protection**

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Do not let product enter drains. Risk of explosion.

---

## **SECTION 9: Physical and chemical properties**

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

- |   |                                     |
|---|-------------------------------------|
| a) Appearance                                   | Form: clear, liquid<br>Color: green |
| b) Odor   | No data available                   |
| c) Odor Threshold                               | No data available                   |
| d) pH   | No data available                   |
| e) Melting point/freezing point                 | No data available                   |
| f) Initial boiling point and boiling range      | No data available                   |
| g) Flash point                                  | -28 °C (-18 °F)                     |
| h) Evaporation rate                             | No data available                   |
| i) Flammability (solid, gas)                    | No data available                   |
| j) Upper/lower flammability or explosive limits | No data available                   |

Aldrich - 779253

Page 6 of 13

|    |   |                              |
|----|---|------------------------------|
| k) | Vapor pressure                            | No data available            |
| l) | Vapor density                             | No data available            |
| m) | Density                                   | No data available            |
|    | Relative density                          | No data available            |
| n) | Water solubility                          | No data available            |
| o) | Partition coefficient:<br>n-octanol/water | No data available            |
| p) | Autoignition<br>temperature               | No data available            |
| q) | Decomposition<br>temperature              | No data available            |
| r) | Viscosity                                 | No data available            |
| s) | Explosive properties                      | Not classified as explosive. |
| t) | Oxidizing properties                      | none                         |

## 9.2 Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Warming.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Mixture

#### Acute toxicity

Oral: No data available

Symptoms: Possible symptoms:, mucosal irritations

Aldrich - 779253

Page 7 of 13

Acute toxicity estimate Dermal - 2,747 mg/kg  
(Calculation method)

**Skin corrosion/irritation**

Remarks: Mixture causes skin irritation.

**Serious eye damage/eye irritation**

Remarks: Mixture causes serious eye irritation.

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

Mixture causes damage to organs through prolonged or repeated exposure.

**Aspiration hazard**

No data available

**11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**Components**

**tert-butyl methyl ether**

**Acute toxicity**

LD50 Oral - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 401)

Symptoms: Nausea, Vomiting, Pulmonary failure possible after aspiration of vomit.,

Aspiration may cause pulmonary edema and pneumonitis.

LC50 Inhalation - Rat - male and female - 4 h - 85 mg/l - vapor

(OECD Test Guideline 403)

Symptoms: Possible damages:, mucosal irritations



LD50 Dermal - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

**Skin corrosion/irritation**

Skin - Rabbit

Result: Skin irritation - 4 h

(OECD Test Guideline 404)

Remarks: Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

**Germ cell mutagenicity**

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: mouse lymphoma cells

Result: negative

Method: OECD Test Guideline 486

Species: Mouse - male and female - Liver cells

Result: negative

Method: US-EPA

Species: Mouse - male and female - Bone marrow

Result: negative

Method: US-EPA

Species: Rat - male and female - Bone marrow

Result: negative

Method: OECD Test Guideline 488

Species: Rat - male - Bone marrow

Result: negative

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

Acute oral toxicity - Nausea, Vomiting, Pulmonary failure possible after aspiration of vomit., Aspiration may cause pulmonary edema and pneumonitis.

Acute inhalation toxicity - Possible damages:, mucosal irritations

## **Specific target organ toxicity - repeated exposure**

### **Aspiration hazard**

No data available

## **1-Azido-4-fluorobenzene**

### **Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

### **Skin corrosion/irritation**

Remarks: No data available

### **Serious eye damage/eye irritation**

Remarks: No data available

### **Respiratory or skin sensitization**

No data available

### **Germ cell mutagenicity**

No data available

### **Carcinogenicity**

No data available

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

---

## **SECTION 12: Ecological information**

### **12.1 Toxicity**

#### **Mixture**

No data available

### **12.2 Persistence and degradability**

No data available

### **12.3 Bioaccumulative potential**

No data available

### **12.4 Mobility in soil**

No data available

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

No data available

### Components

#### tert-butyl methyl ether

|   |  |
|---|--|
| Toxicity to fish  | semi-static test LC50 - Menidia beryllina - 574 mg/l - 96 h (OECD Test Guideline 203)              |
| Toxicity to daphnia and other aquatic invertebrates                   | flow-through test EC50 - Americamysis bahia (Mysid) - 187 mg/l - 96 h (US-EPA OPPTS 850.1035)      |
| Toxicity to algae   | static test IC50 - Pseudokirchneriella subcapitata (green algae) - 491 mg/l - 96 h                 |
| Toxicity to bacteria  | static test EC10 - Pseudomonas putida - 710 mg/l - 18 h<br>Remarks: (ECHA)                         |
| Toxicity to fish(Chronic toxicity)                                    | flow-through test NOEC - Pimephales promelas (fathead minnow) - 299 mg/l - 31 d<br>Remarks: (ECHA) |
|   | flow-through test NOEC - Pimephales promelas (fathead minnow) - 450 mg/l - 31 d<br>Remarks: (ECHA) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | flow-through test NOEC - Daphnia magna (Water flea) - 51 mg/l - 21 d (OPPTS 850.1300)              |

#### 1-Azido-4-fluorobenzene

No data available

---

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

---

## SECTION 14: Transport information

#### DOT (US)

UN number: 2398    Class: 3    Packing group: II  
Proper shipping name: Methyl tert-butyl etherSOLUTION

Reportable Quantity (RQ): 1098 lbs  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2398    Class: 3    Packing group: II    EMS-No: F-E, S-D  
Proper shipping name: METHYL tert-BUTYL ETHERSOLUTION

#### IATA

UN number: 2398    Class: 3    Packing group: II  
Proper shipping name: Methyl tert-butyl etherSOLUTION

---

## SECTION 15: Regulatory information

#### CERCLA Reportable Quantity

| Components              | CAS-No.   | Component RQ (lbs) | Calculated product RQ (lbs) |
|-------------------------|-----------|--------------------|-----------------------------|
| tert-butyl methyl ether | 1634-04-4 | 1000               | 1098                        |

#### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

#### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313** : The following components are subject to reporting levels established by SARA Title III, Section 313:

|              |           |                  |
|--------------|-----------|------------------|
| tert-butyl   | 1634-04-4 | >= 90 - <= 100 % |
| methyl ether |           |                  |

#### US State Regulations

##### Massachusetts Right To Know

|   |   |
|---|---|
| tert-butyl methyl ether   | 1634-04-4   |
| <b>Massachusetts Right To Know</b>  |   |
| tert-butyl methyl ether   | 1634-04-4   |
| <b>Pennsylvania Right To Know</b>   |   |
| tert-butyl methyl ether   | 1634-04-4   |
| 1-Azido-4-fluorobenzene   | 3296-02-4   |
| <b>Pennsylvania Right To Know</b>   |   |
| tert-butyl methyl ether   | 1634-04-4   |
| <b>Maine Chemicals of High Concern</b>  |   |
| tert-butyl methyl ether   | 1634-04-4   |
| <b>Vermont Chemicals of High Concern</b>  |   |
| Product does not contain any listed chemicals                                     |   |
| <b>Washington Chemicals of High Concern</b>                                       |   |
| Product does not contain any listed chemicals                                     |   |
| <b>New Jersey Right To Know</b>   |   |
| tert-butyl methyl ether   | 1634-04-4   |
| 1-Azido-4-fluorobenzene   | 3296-02-4   |
| <b>The ingredients of this product are reported in the following inventories:</b> |   |
| TSCA  | : Product contains substance(s) not listed on TSCA inventory. |

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

---

## **SECTION 16: Other information**

### **Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 8.7

Revision Date: 09/07/2024

Print Date: 09/08/2024