SAFETY DATA SHEET

Version 6.6
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 4-Azidobenzoic acid solution

Product Number : 778877
Brand : Aldrich
Index-No. : 603-181-00-X
CAS-No. : 1634-04-4

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
Specific target organ toxicity - repeated exposure (Category 1), Blood, H372

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

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H315	Causes skin irritation.
H372	Causes damage to organs (Blood) 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 mist or vapors.
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.
P314	Get medical advice/ attention if you feel unwell.
P332 + P313	If skin irritation occurs: 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 : p-Azidobenzoic acid solution

Formula : C5H12O
Molecular weight : 163.13 g/mol

Component		Classification	Concentration
tert-butyl methyl ether			
CAS-No. EC-No.	1634-04-4 216-653-1	Flam. Liq. 2; Skin Irrit. 2; H225, H315	<= 100 %

Index-No. Registration number	603-181-00-X 01-2119452786-27-XXXX		
4-azidobenzoic acid			
CAS-No. EC-No.	6427-66-3 229-198-9	B; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; STOT RE 1; H241, H315, H319, H335, H372	>= 1 - < 5 %

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 (NOx)
Combustible.

Pay attention to flashback.
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.
Storage stability Recommended storage temperature

2 - 8 °C
Light sensitive.

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 144 mg/m3	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 entrepeneur 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 Color: light green, light yellow
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	No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	0.769 g/cm3
	Relative density	No data available

n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	No data available
q)	Decomposition 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
No data available

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
Acute toxicity estimate Oral - 2,551 mg/kg
(Calculation method)
LD50 Oral - Rat - male and female - > 2,000 mg/kg (tert-butyl methyl ether)
(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
(tert-butyl methyl ether)

(OECD Test Guideline 403)
Symptoms: Possible damages:, mucosal irritations
Acute toxicity estimate Dermal - 2,551 mg/kg
(Calculation method)
LD50 Dermal - Rat - male and female - > 2,000 mg/kg (tert-butyl methyl ether)
(OECD Test Guideline 402)

Skin corrosion/irritation
Remarks: Mixture causes skin irritation.
Skin - Rabbit (tert-butyl methyl ether)
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 (tert-butyl methyl ether)
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig (tert-butyl methyl ether)
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: In vitro mammalian cell gene mutation test
(tert-butyl methyl ether)
Test system: Chinese hamster lung cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Ames test
(tert-butyl methyl ether)
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: Mutagenicity (mammal cell test): micronucleus.
(tert-butyl methyl ether)
Test system: mouse lymphoma cells
Metabolic activation: without metabolic activation
Method: OECD Test Guideline 473
Result: negative
(tert-butyl methyl ether)
Test Type: unscheduled DNA synthesis assay
Species: Mouse
Cell type: Liver cells
Application Route: inhalation (vapor)
Method: OECD Test Guideline 486
Result: negative
(tert-butyl methyl ether)
Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow

Application Route: inhalation (vapor)
Method: US-EPA
Result: negative
(tert-butyl methyl ether)
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Species: Rat
Cell type: Bone marrow
Application Route: inhalation (vapor)
Method: US-EPA
Result: negative
(tert-butyl methyl ether)
Test Type: Transgenic rodent somatic cell gene mutation assay
Species: Rat
Cell type: Bone marrow
Application Route: inhalation (vapor)
Method: OECD Test Guideline 488
Result: negative

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.
- Blood

Aspiration hazard
No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 3,000 mg/kg
Remarks: Subchronic toxicity
(tert-butyl methyl ether)
Nausea, Vomiting, Dizziness, Central nervous system depression, Aspiration or inhalation may cause chemical pneumonitis., MTBE (methyl-tert-butyl ether) is reported to metabolize to tert-butyl alcohol and formaldehyde by microsomal demethylation, MTBE (methyl-tert-butyl ether) should be considered a "potential human carcinogen" due to an increase in leydig interstitial cell tumors of testes in male rats and an increase in lymphomas, leukemias, and uterine sarcomas in female rats., In another unpublished study MTBE was shown to be carcinogenic due to "increased incidence of a rare type of kidney tumor" in male rats and an "increase in the incidence of hepatocellular adenomas" in female mice.
(tert-butyl methyl ether)

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (tert-butyl methyl ether)

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Systemic effects:
(tert-butyl methyl ether)
After absorption of large quantities:
(tert-butyl methyl ether)
somnolence
Dizziness
agitation, spasms
CNS disorders
narcosis
Unconsciousness
(tert-butyl methyl ether)
Other dangerous properties can not be excluded.
(tert-butyl methyl ether)
Handle in accordance with good industrial hygiene and safety practice.
(tert-butyl methyl ether)

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

4-azidobenzoic acid

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
May cause respiratory irritation. - Upper respiratory tract

Specific target organ toxicity - repeated exposure
Causes damage to organs through prolonged or repeated exposure.
- Blood

Aspiration hazard
No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture

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

toxicity)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d (tert-butyl methyl ether) Result: 0 % - Not readily biodegradable. (OECD Test Guideline 301D)

12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 28 d at 25 °C(tert-butyl methyl ether) Bioconcentration factor (BCF): 1.5

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 Remarks: (ECHA)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 299 mg/l - 31 d Remarks: (ECHA)
	flow-through test NOEC - Pimephales promelas (fathead minnow) - 450 mg/l - 31 d 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)

4-azidobenzoic acid

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): 1020 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	1020

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

US State Regulations

Massachusetts Right To Know

tert-butyl methyl ether 1634-04-4

Pennsylvania Right To Know

tert-butyl methyl ether 1634-04-4

Maine Chemicals of High Concern

tert-butyl methyl ether 1634-04-4

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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