

SAFETY DATA SHEET

Version 6.12
Revision Date 03/04/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Anisole
Product Number : 296295
Brand : Sigma-Aldrich
CAS-No. : 100-66-3

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 3), H226
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
Short-term (acute) aquatic hazard (Category 3), H402

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

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2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Warning

Hazard Statements

H226

Flammable liquid and vapor.

H336

May cause drowsiness or dizziness.

H402

Harmful to aquatic life.

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.

P261

Avoid breathing mist or vapors.

P271

Use only outdoors or in a well-ventilated area.

P273

Avoid release to the environment.

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.

P304 + P340 + P312

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P370 + P378

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

P403 + P233

Store in a well-ventilated place. Keep container tightly closed.

P403 + P235

Store in a well-ventilated place. Keep cool.

P405

Store locked up.

P501

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

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Repeated exposure may cause skin dryness or cracking.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Methoxybenzene
Methyl phenyl ether

Formula : C₇H₈O
Molecular weight : 108.14 g/mol
CAS-No. : 100-66-3
EC-No. : 202-876-1

Component	Classification	Concentration
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Anisole		
	Flam. Liq. 3; STOT SE 3; Aquatic Acute 3; H226, H336, H402	<= 100 %

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.

In case of eye contact

After eye contact: rinse out with plenty of water. 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

Carbon dioxide (CO₂) Foam 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

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Remove container from danger zone and cool with water. 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 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

Change contaminated clothing. Wash hands 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.

hygroscopic Handle and store under inert gas.

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

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands 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

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

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

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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: liquid, clear
Color: colorless |
| b) Odor | sweet |
| c) Odor Threshold | No data available |
| d) pH | at 20 °C (68 °F) Not applicable |
| e) Melting point/freezing point | Melting point/range: -37 °C (-35 °F) |
| f) Initial boiling point and boiling range | 155 °C 311 °F |
| g) Flash point | 51.7 °C (125.1 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 6.3 %(V)
Lower explosion limit: 0.34 %(V) |
| k) Vapor pressure | 13.33 hPa at 42.20 °C (107.96 °F) |
| l) Vapor density | 3.73 - (Air = 1.0) |
| m) Density | 0.995 g/cm ³ at 20 °C (68 °F) |
| Relative density | No data available |
| n) Water solubility | 1.71 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - soluble |
| o) Partition coefficient: n-octanol/water | log Pow: 2.62 at 30 °C (86 °F) - Bioaccumulation is not expected. |
| p) Autoignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

Relative vapor 3.73 - (Air = 1.0)

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density

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Strong acids

alkalines

formaldehyde

10.4 Conditions to avoid

Heating.

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

Acute toxicity

LD50 Oral - Rat - 3,700 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

Gastrointestinal:Changes in structure or function of salivary glands.

Kidney, Ureter, Bladder:Hematuria.

(RTECS)

LC50 Inhalation - Rat - male and female - 4 h - > 6.51 mg/l - vapor

(OECD Test Guideline 403)

Dermal: No data available

Dermal: Repeated exposure may cause skin dryness or cracking.

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

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(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

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

Inhalation - May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Ingestion of large amounts may cause: , bladder effects, Liver injury may occur., Kidney injury may occur., It has a narcotic action and acts as a depressant on the central nervous system.

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

Systemic effects:

After uptake of large quantities:

Nausea
Vomiting
agitation, spasms
Headache
muscle twitching
narcosis
cardiovascular disorders

Possible damages:

Damage to:

Liver
Kidney
Central nervous system

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Danio rerio (zebra fish) - > 1 mg/l - 96 h Remarks: (ECOTOX Database)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (algae) - 47 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test NOEC - activated sludge - 300 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 14 d Result: 56 % - Readily biodegradable. (OECD Test Guideline 301C)
Theoretical oxygen demand	2,520 mg/g Remarks: (Lit.)

12.3 Bioaccumulative potential

Bioaccumulation	Gambusia affinis (Mosquito fish) - 24 h - 8.54 µg/l (Anisole)
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Bioconcentration factor (BCF): 22

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

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 2222 Class: 3 Packing group: III
Proper shipping name: Anisole
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2222 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: ANISOLE

IATA

UN number: 2222 Class: 3 Packing group: III
Proper shipping name: Anisole

SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

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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