

4-Allylanisole SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: 4-Allylanisole
- * Catalog Number: S5339
- * CAS Number: 140-67-0
- * IUPAC Name: Benzene, 1-methoxy-4-(2-propen-1-yl)-

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Flammable liquids: Category 4. H227
- Acute toxicity (oral): Category 4. H302
- Skin irritation: Category 2. H315
- Skin sensitization: Category 1. H317
- Germ cell mutagenicity: Category 2. H341
- Carcinogenicity: Category 2. H351
- Chronic aquatic toxicity: Category 3. H412

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Warning

Hazard statement(s)

- H227: Combustible liquid
- H302: Harmful if swallowed
- H315: Causes skin irritation
- H317: May cause an allergic skin reaction
- H341: Suspected of causing genetic defects
- H351: Suspected of causing cancer
- H412: Harmful to aquatic life with long lasting effects

Precautionary statement(s)	None.
Prevention	P203: Obtain, read and follow all safety instructions before use. P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. No smoking. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P272: Contaminated work clothing should not be allowed out of the workplace. P273: Avoid release to the environment. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P317: IF SWALLOWED: Get medical help. P302+P352: IF ON SKIN: wash with plenty of water. P318: if exposed or concerned, get medical advice. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P332+P317: If skin irritation occurs: Get medical help. P333+P317: If skin irritation or rash occurs: Get medical help. P362+P364: Take off contaminated clothing and wash it before reuse. P370+P378: In case of fire: Use water spray, dry chemical, carbon dioxide, or appropriate foam to extinguish.
Storage	P403: Store in a well-ventilated place. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: 4-Allylanisole

CAS Number: 140-67-0

PubChem CID: 8815

Molecular formula: C₁₀H₁₂O

Molecular weight: 148.20 g/mol

IUPAC name: 1-methoxy-4-prop-2-enylbenzene

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to t

Skin contact: SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

Eye contact: EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician.

IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

Ingestion: INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Fires involving this compound should be controlled using a dry chemical, carbon dioxide, foam or halon extinguisher. (NTP, 1992)

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Unsuitable extinguishing media: Do NOT use water jet.

Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Use water spray to cool unopened containers.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 178 °F (NTP, 1992)

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Methods and materials for containment and cleaning up: Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations. Keep in suitable, closed containers for disposal.

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber; **Contaminated packaging:** Dispose of as unused product.

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Precautions for safe handling: Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

SRP: The scientific literature for the use of contact lenses by industrial workers is inconsistent. The benefits or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: If you spill this chemical, use absorbent paper to pick up all liquid spill material. Your contaminated clothing and absorbent paper should be sealed in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with alcohol followed by washing with a strong soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should store this material in a refrigerator. (NTP, 1992)

Keep container tightly closed in a dry and well-ventilated place.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

Store in original container. Keep upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear safety glasses with side shields.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Estragole is a colorless liquid with odor of anise. Insoluble in water. Isolated from rind of persea gratissima grath. and from oil of estragon. Found in oils of Russian anise, basil, fennel turpentine, tarragon oil, anise bark oil. (NTP, 1992)

- b) Odor: Odor reminiscent of anise with a corresponding sweet taste (differing from anethole)
- 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: 421 °F at 764 mmHg (NTP, 1992)
- g) Flash point: 178 °F (NTP, 1992)
- 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: 0.05 [mmHg]
- l) Vapor density: No data available
- m) Relative density: 0.9645 at 70 °F (NTP, 1992) - Less dense than water; will float
- n) Water solubility: Insoluble (<1 mg/ml) (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 3.4
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 9.2 Å²
Complexity: 112

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂).
See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

Causes skin irritation (H315).

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

Germ cell mutagenicity:

Suspected of causing genetic defects (H341).

Carcinogenicity:

Suspected of causing cancer (H351).

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.

11.2 Additional information

No additional toxicological information available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

1-Methoxy-4-(2-propenyl)benzene's production and use as flavoring in foods and liqueurs may result in its release to the environment through various waste streams; its use in fragrances will result in its direct release to the environment. 1-Methoxy-4-(2-propenyl)benzene is found in many plants, in particular spices. If released to air, an estimated vapor pressure of 0.17 mm Hg at 25 °C indicates 1-methoxy-4-(2-propenyl)benzene will exist solely as a vapor in the atmosphere. Vapor-phase 1-methoxy-4-(2-propenyl)benzene will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 7 hrs. 1-Methoxy-4-(2-propenyl)benzene does not contain chromophores that absorb at wavelengths >290 nm and, therefore, is not expected to be susceptible to direct photolysis by sunlight. If released to soil, 1-methoxy-4-(2-propenyl)benzene is expected to have low mobility based upon an estimated Koc of 520. Volatilization from moist soil surfaces is expected to be an important fate process based upon an estimated Henry's Law constant of 4.6×10^{-4} atm-cu m/mole. 1-Methoxy-4-(2-propenyl)benzene has an estimated vapor pressure of 0.17 mm Hg and exists as a liquid under environmental conditions; therefore, 1-methoxy-4-(2-propenyl)benzene may volatilize from dry soil. Utilizing the OECD 301F ready Biodegradability test, 48% O₂ consumption was reached in 4 weeks indicating that biodegradation may be an important envi

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 3.4

Potential for bioaccumulation exists (Log P > 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

This substance is classified as hazardous to the aquatic environment.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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:

Acute (short-term) health hazard

Chronic (long-term) health hazard

Environmental hazard

Fire hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: Benzene, 1-methoxy-4-(2-propenyl)-
- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity Authoritative List - Prop 65 Report - regardless of intended function of ingredient in the product
- EFSA Legal Basis: Regulation (EC) No 1831/2003 (amended)
- FDA Requirements: Synthetic flavoring substances and adjuvants may be safely used in food in accordance with the following conditions. (a) They are used in the minimum quantity required to produce their intended effect, and otherwise in accordance with all the principles of good manufacturing practice. (b) They consi

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.