cis-Anethole SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: cis-Anethole
* Catalog Number: S3779
* CAS Number: 104-46-1
* IUPAC Name: Benzene, 1-methoxy-4-(1-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):

Skin sensitization: Category 1. H317

Chronic aquatic toxicity: Category 3. H412

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)	
Signal Word	Warning
Hazard statement(s)	H317: May cause an allergic skin reaction H412: Harmful to aquatic life with long lasting effects
Precautionary statement(s)	None.
Prevention	P261: Avoid breathing dust/fume/gas/mist/vapors/spray. 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	P302+P352: IF ON SKIN: wash with plenty of water. P321: Specific treatment (see information on this label and safety datasheet)). P333+P317: If skin irritation or rash occurs: Get medical help. P362+P364: Take off contaminated clothing and wash it before reuse.
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: cis-Anethole

CAS Number: 104-46-1

PubChem CID: 637563

Molecular formula: C10H12O

Molecular weight: 148.20 g/mol

IUPAC name: 1-methoxy-4-[(E)-prop-1-enyl]benzene

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

To extinguish a fire involving this chemical you may use a dry chemical, carbon dioxide, foam or halon extinguisher; a water spray may also be used. (NTP, 1992)

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: 195 °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

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: Use absorbent paper to pick up spill material. Contaminated clothing and absorbent paper should be sealed in a vapor-tight plastic bag for eventual disposal. Solvent-wash contaminated surfaces with alcohol followed by washing with a strong soap and water solution.

STORAGE PRECAUTIONS: You should keep this material in a tightly-closed container under an inert atmosphere, and store it at refrigerated temperatures. (NTP, 1992)

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

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: Anethole appears as white crystals or a liquid. Odor of anise oil and a sweet taste. (NTP, 1992)

b) Odor: ANISE OIL ODOR

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 70.4 °F (NTP, 1992)

f) Initial boiling point and boiling range: 454.1 °F at 760 mmHg (NTP, 1992)
g) Flash point: 195 °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: 0.9882 (NTP, 1992) - Less dense than water; will float
n) Water solubility: Slightly soluble (NTP, 1992)
o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 3.3
p) Auto-ignition temperature: No data available
q) Decomposition temperature: No data available
r) Viscosity: 2.45X10-3 Pa.s
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: 121

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

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO□).
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:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

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.

11.2 Additional information

No additional toxicological information available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Anethole occurs naturally in anise, star anise, and fennel oils and chickpea seed. Anethole's use as an insect attractant, and in perfumery, soap and dentifrices, and color photography could result in its release to the environment through various waste streams. Anethole has been found in three studies of effluent samples. Insufficient data are available to predict the relative importance or rate of biodegradation in soil or water. Anethole is expected to have medium to low mobility in soil. In water, anethole is expected to volatilize and have some adsorption to suspended solids and sediment. Anethole will exist in the vapor phase in the ambient atmosphere. If released to the atmosphere, it will degrade by reaction with photochemically produced radicals with estimated half-lives of approximately 4.9 and 4.5 hours for the cis and trans isomers, respectively. Anethole will also degrade by reaction with atmospheric ozone with estimated half-lives for the cis and trans isomers of 4.03 and 2.02 hours, respectively. The general population is exposed to anethole through consumption of foodstuffs. (SRC)

Anethole occurs naturally in anise, star anise, and fennel oils(1) and chickpea seed(2).

Chloronitrobenzenes are produced by nitration of chlorobenzene. The crude chloronitrobenzene obtained from the nitration process contains about 34% o-chloronitrobenzene, 65% p-chloronitrobenzene, and 1% m-chloronitrobenzene. The isomers are separated by a combination of crystallization and distil

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 3.3

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).

DOT label: Combustible Liquid

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

Environmental 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-(1-propenyl)-
- The Australian Inventory of Industrial Chemicals: Chemical: Benzene, 1-methoxy-4-(1-propenyl)-, (E)-
- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Fragrance Allergen Authoritative List - Annex III of the EU Cosmetics Regulation No. 1223/2009 - Fragrance Allergens Report - if present in a rinse-off cosmetic product at a concentrat
- EFSA Legal Basis: Regulation (EC) No 1831/2003 (amended)
- Status Regulation (EC): 2007/442

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.