

Pulegone SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Pulegone

* Catalog Number: S9140

* CAS Number: 89-82-7

* IUPAC Name: Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (5R)-

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):

Acute toxicity (oral): Category 3. H301

Acute toxicity (oral): Category 4. H302

Carcinogenicity: Category 2. H351

Specific target organ toxicity (repeated exposure): Category 1. H372

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H301: Toxic if swallowed

H302: Harmful if swallowed

H351: Suspected of causing cancer

H372: Causes damage to organs through prolonged or repeated exposure

Precautionary statement(s)

None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P260: Do not breathe dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P301+P317: IF SWALLOWED: Get medical help. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth.
Storage	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: Pulegone

CAS Number: 89-82-7

PubChem CID: 442495

Molecular formula: C₁₀H₁₆O

Molecular weight: 152.23 g/mol

IUPAC name: (5R)-5-methyl-2-propan-2-ylidenecyclohexan-1-one

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

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

Wear self contained breathing apparatus for fire fighting if necessary. /(R)-(+)-Pulegone/

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. /(R)-(+)-Pulegone/

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.

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.

WARNING: Highly toxic — only trained personnel should handle spills.

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. /(R)-(+)-Pulegone/

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. /(R)-(+)-Pulegone/

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. /(R)-(+)-Pulegone/

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. /(R)-(+)-Pulegone/

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: Liquid with a pleasant odor between peppermint and camphor; [Merck Index] Clear light brown liquid; [Sigma-Aldrich MSDS]

b) Odor: Pleasant odor, midway between peppermint and camphor

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: < 25 °C

f) Initial boiling point and boiling range: 224 °C

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: 138.0 [mmHg]

- l) Vapor density: No data available
- m) Relative density: 0.9323 at 20 °C
- n) Water solubility: Practically insoluble in water
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2.8
- 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): 17.1 Å²
Complexity: 197

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. /(R)-(+)-Pulegone/
/Conditions to avoid/ Heat, flames and sparks. /(R)-(+)-Pulegone/

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:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

Suspected of causing cancer (H351).

Reproductive toxicity:

No data available.

Specific target organ toxicity (single exposure):

H372

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

Pulegone

Group 2B: Possibly carcinogenic to humans

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Pulegone

TR-563: Toxicology and Carcinogenesis Studies of Pulegone (CASRN 89-82-7) in F344/N Rats and B6C3F1 Mice (Gavage Studies) (2011)

11/19/09

No Evidence

Some Evidence

Clear Evidence

Clear Evidence

Under the conditions of these 2-year gavage studies, there was no evidence of carcinogenic activity of pulegone in male F344/N rats administered 18.75, 37.5, or 75 (stop-exposure) mg/k

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

EC50; Species: Daphnia pulex (Water Flea) age <24 hr, neonate; Conditions: freshwater, static, 17 °C, hard water; Concentration: 24400 ug/L for 48 hr; Effect: intoxication, immobilization /> or = 96% purity/

Pulegone's production and use as a chemical intermediate, flavoring and herbal medication may result in its release to the environment through various waste streams. The compound is a ketone found in oils derived from plants of the Labiarae family. If released to air, an estimated vapor pressure of 0.12 mm Hg at 25 °C indicates pulegone will exist solely as a vapor in the atmosphere. Vapor-phase pulegone 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 0.1 days. Pulegone contains chromophores that absorb at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, pulegone is expected to have moderate mobility based upon an estimated Koc of 670. Volatilization from moist soil surfaces may be an important fate process based upon an estimated

Henry's Law constant of 5.9×10^{-5} atm-cu m/mole. Pulegone may volatilize from dry soil surfaces based upon its vapor pressure. Biodegradation data in soil or water were not available. If released into water, pulegone is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is expected to be an important fate process base

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2.8

Low potential for bioaccumulation ($\text{Log P} < 3$).

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

No other adverse ecological effects identified.

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: Not available in public databases.

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

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: Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)-
- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity Authoritative List - IARC Carcinogens - 2B; Prop 65 Report - regardless of intended function of ingredient in the product
- EFSA Legal Basis: Regulation (EC) No 178/2002 (amended)
- FDA Requirements: Pulegone is a food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant 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

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: 2026/09/10

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.