

Dehydroacetic acid SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Dehydroacetic acid
- * Catalog Number: S4522
- * CAS Number: 520-45-6
- * IUPAC Name: 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl-

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 4. H302

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word Warning

Hazard statement(s) H302: Harmful if swallowed

Precautionary statement(s) None.

Prevention P264: Wash hands thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.

Response P301+P317: IF SWALLOWED: Get medical help.
P330: Rinse mouth.

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: Dehydroacetic acid

CAS Number: 520-45-6

PubChem CID: 122903

Molecular formula: C₈H₈O₄

Molecular weight: 168.15 g/mol

IUPAC name: 3-acetyl-6-methylpyran-2,4-dione

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

WATER OR FOAM MAY CAUSE FROTHING.

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: 157 °C; 315 °F (OPEN CUP)

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

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

Handle in accordance with good industrial hygiene and safety practices.

Wear appropriate PPE (see Section 8). Avoid contact with skin, eyes, and clothing.

Wash hands thoroughly after handling. Do not eat, drink, or smoke in work area.

Avoid dust formation. Use only in a chemical fume hood or well-ventilated area.

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).]

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: Dry Powder
- b) Odor: ODORLESS
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 109-111 °C (SUBLIMES)
- f) Initial boiling point and boiling range: 269.9 °C @ 760 MM HG
- g) Flash point: 157 °C; 315 °F (OPEN CUP)
- 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: 1.9 MM HG AT 100 °C
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: (WT/WT) 22% IN ACETONE, 18% IN BENZENE, 5% IN METHANOL, 3% IN USP ETHANOL, 3% IN CARBON TETRACHLORIDE, 5% IN ETHER, 0.7% IN N-HEPTANE, LESS THAN 0.1% IN GLYCEROL, 1.6% IN OLIVE OIL, 1.7% IN PROPYLENE GLYCOL, LESS THAN 0.1% IN WATER AT 25 °C
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 0.3
- p) Auto-ignition temperature: 366 °C (690 °F)
- 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): 60.4 Å²

Complexity: 287

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

HIGHLY REACTIVE

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:

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

Dehydroacetic acid's production and use in organic syntheses, as a plasticizer, bactericide, in anti-enzyme toothpastes, and as a fungicide in cosmetics and on processed fruits and vegetables may result in its release to the environment. If released to the atmosphere, dehydroacetic acid is expected to exist solely in the vapor phase in the ambient atmosphere based on an extrapolated vapor pressure of 1.1×10^{-3} mm Hg at 25 °C. Vapor-phase dehydroacetic acid is degraded in the atmosphere by reaction with ozone and photochemically-produced hydroxyl radicals with an estimated half-life of about 1.0 day and 4.9 hours, respectively. If released to soil, an estimated Koc of 120 suggests that dehydroacetic acid will have high mobility in soil. Volatilization from moist and dry soil surfaces is not expected to be important based on an estimated Henry's Law constant of 3.4×10^{-7} atm-cu m/mole at 25 °C and the extrapolated vapor pressure for this compound, respectively. Biodegradation of dehydroacetic acid in water and soil is expected to be an important removal process based upon aqueous screening studies. If released into water, an estimated Koc of 120 indicates that dehydroacetic acid is not expected to adsorb to suspended solids and sediment in the water column. The potential for bioconcentration in aquatic organisms is low based on an estimated BCF of 15. Volatilization of dehydroacetic acid from water surfaces is not expected to be an important fate based on the estimated Henry's La

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 0.3

Low potential for bioaccumulation (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: 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

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: 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl-
- FDA Requirements: Dehydroacetic acid is a food additive permitted for direct addition to food for human consumption, as long as 1) the quantity added to food does not exceed the amount reasonably required to accomplish its intended physical, nutritive, or other technical effect in food, and 2) when intended for use i

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.