

4-oxo-2-Nonenal-d3

Cayman Chemical Company
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108

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1. Product and Company Identification

Product Code: 10004174
Product Name: 4-oxo-2-Nonenal-d3
Manufacturer Information
Company Name: Cayman Chemical Company
Emergency Contact: Cayman Chemical Company (800)364-9897
Information: Cayman Chemical Company (734)971-3335
Chemical Family: Autoxidation
Synonyms: (+/-)-4-hydroxy-2E-nonenal-d3; 4-ONE-d3

2. Composition/Information on Ingredients

Hazardous Components (Chemical Name)	CAS #	Percentage	OSHA PEL	ACGIH TWA	Other Limits
1. 4-oxo-2-Nonenal-d3	NA	0.05 %	No data.	No data.	No data.
2. Methyl acetate	79-20-9	99.95 %	8H TWA:200 ppm (610 mg/m3)	200 ppm	No data.

Hazardous Components (Chemical Name)	RTECS #	OSHA STEL	OSHA CEIL	ACGIH STEL	ACGIH CEIL
1. 4-oxo-2-Nonenal-d3	NA	No data.	No data.	No data.	No data.
2. Methyl acetate	A19100000	No data.	No data.	250 ppm	No data.

3. Hazards Identification

Emergency Overview: No data available.
Route(s) of Entry: Inhalation? Yes Skin? Yes Eyes? Yes Ingestion? Yes Other: Injection
Potential Health Effects (Acute and Chronic): The hazards identified with this product are those associated with the solvent(s).
 Material is irritating to the mucous membranes and upper respiratory tract.
 May be harmful by inhalation, ingestion, or skin absorption.
 May cause eye, skin, or respiratory system irritation.
 Repeated exposure may cause skin dryness or cracking.
 The toxicological properties of this compound have not been fully evaluated.
 Vapors may cause drowsiness and dizziness.
LD 50/LC 50: Please refer to Section 11.
Signs and Symptoms Of Exposure: Irritating to the skin, eyes, nose, throat, and respiratory tract.
 Methyl acetate is metabolized into formic acid. Humans and other primates metabolize formic acid more slowly than do rodents. Formic acid can build up in the body producing toxic effects possibly leading to death; therefore data from studies in rodents may have limited relevance for human risk assessment.

4. First Aid Measures

Emergency and First Aid Procedures: If inhaled remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.
 If swallowed, wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.
 In case of contact with eyes, hold eyelids apart and flush eyes with plenty of water. After initial flushings, remove any contact lenses and continue flushing for at least 20 minutes. Have eyes examined and tested by medical personnel.
 In case of skin contact, immediately wash skin with soap and plenty of water. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

5. Fire Fighting Measures

Flash Pt: -10.00 C Method Used: closed cup

Explosive Limits: LEL: 3.1% at 25.0 C UEL: 16% at 25.0 C

Autoignition Pt: 502.00 C

Fire Fighting Instructions: As in any fire, wear self-contained breathing apparatus pressure-demand (MSHA/NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.
Note: Flammable as diluted in methyl acetate

Flammable Properties and Hazards: Can release vapors that form explosive mixtures at temperatures at or above the flash point.
Container explosion may occur under fire conditions.
Emits toxic fumes under fire conditions.
Flammable liquid.
Vapors can travel to a source of ignition and flash back.

Extinguishing Media: Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray when fighting fires involving this material.
Use of water spray when fire fighting may be inefficient.
Use water spray to cool fire-exposed containers.

6. Accidental Release Measures

Steps To Be Taken In Case Material Is Released Or Spilled: Wear a government approved respirator and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
Absorb spill with inert material (e.g. dry sand or earth), then place in a chemical waste container.
After removal, ventilate contaminated area and flush thoroughly with water.

7. Handling and Storage

Hazard Label Information: Avoid contact with skin and eyes. Do not reuse this container. Use with adequate ventilation.
Wash thoroughly after handling.

Precautions To Be Taken in Handling: Avoid breathing (dust, vapor, mist, gas).
Avoid contact with eyes, skin, and clothing.
Avoid prolonged or repeated exposure.
Do not reuse this container.
Keep away from sources of ignition.
Use with adequate ventilation.
Wash thoroughly after handling.

Precautions To Be Taken in Storing: Keep tightly closed.
Store at correct temperature.

Other Precautions: Protect from moisture.

8. Exposure Controls/Personal Protection

Protective Equipment Summary - Hazard Label Information: Eye wash station in work area Lab coat Protective gloves Safety glasses Safety shower in work area Vent Hood

Respiratory Equipment (Specify Type): Government approved respirator as conditions warrant.

Eye Protection: Safety glasses

Protective Gloves: Use appropriate hand protection based on solvent.

Other Protective Clothing: Lab coat

Engineering Controls (Ventilation etc.): Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

Work/Hygienic/Maintenance Practices: Do not take internally.
Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower.
Wash thoroughly after handling.

9. Physical and Chemical Properties

Physical States:	[] Gas [X] Liquid [] Solid
Melting Point:	No data.
Boiling Point:	No data.
Specific Gravity (Water = 1):	No data.
Vapor Pressure (vs. Air or mm Hg):	165 MM_HG at 20.0 C
Vapor Density (vs. Air = 1):	No data.
Evaporation Rate (vs Butyl Acetate=1):	No data.
Solubility in Water:	0.5 mg/ml* at 25.0 C
Other Solubility Notes:	*PBS pH 7.2, sol. in EtOH, DMSO, & DMF
Percent Volatile:	No data.
Formula:	C9H11D3O2
Molecular Weight:	157.20
pH:	No data.
Appearance and Odor:	A clear, colorless solution

10. Stability and Reactivity

Stability:	Unstable [] Stable [X]
Conditions To Avoid - Instability:	protect from moisture
Incompatibility - Materials To Avoid:	strong oxidizing agents
Hazardous Decomposition Or Byproducts:	carbon dioxide carbon monoxide
Hazardous Polymerization:	Will occur [] Will not occur [X]
Conditions To Avoid - Hazardous Polymerization:	No data available.

11. Toxicological Information

Toxicological Information:	The toxicological effects of this compound have not been thoroughly studied.
	Methyl Acetate - Toxicity Data: Oral LD50 (rat): > 5000 mg/kg Oral LD50 (rabbit): 3705 mg/kg Skin LD50 (rabbit): > 5000 mg/kg
	Methyl Acetate - Irritation Data: Skin (rabbit): 500 mg 24H mild effect Skin (rabbit): 20 mg 24H moderate effect Eyes (rabbit): 100 mg 24H moderate effect
Chronic Toxicological Effects:	Methyl Acetate - Investigated as a tumorigen, mutagen, and reproductive effector. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Methyl Acetate RTECS Number: AI9100000
Carcinogenicity/Other Information:	No data available.
Carcinogenicity:	NTP? No IARC Monographs? No OSHA Regulated? No

12. Ecological Information

Ecological Information:	Runoff from fire control or dilution water may cause pollution.
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13. Disposal Considerations

Waste Disposal Method:	Dispose in accordance with local, state, and federal regulations.
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14. Transport Information

LAND TRANSPORT (US DOT)

DOT Proper Shipping Name: Methyl acetate
DOT Hazard Class: 3
DOT Hazard Label: Flammable Liquid
UN/NA Number: 1231
DOT Packing Group: II
Additional Transport Information: Transport in accordance with local, state, and federal regulations.

15. Regulatory Information

US EPA SARA Title III

Hazardous Components (Chemical Name)	CAS #	Sec.302 (EHS)	Sec.304 RQ	Sec.313 (TRI)	Sec.110
1. 4-oxo-2-Nonenal-d3	NA	No	No	No	No
2. Methyl acetate	79-20-9	No	No	No	No

US EPA CAA, CWA, TSCA

Hazardous Components (Chemical Name)	CAS #	EPA CAA	EPA CWA NPDES	EPA TSCA	CA PROP 65
1. 4-oxo-2-Nonenal-d3	NA	No	No	No	No
2. Methyl acetate	79-20-9	No	No	8A PAIR ,8D	No

SARA (Superfund Amendments and Reauthorization Act of 1986) Lists:

Sec.302: EPA SARA Title III Section 302 Extremely Hazardous Chemical with TPQ. * indicates 10000 LB TPQ if not volatile.
Sec.304: EPA SARA Title III Section 304: CERCLA Reportable + Sec.302 with Reportable Quantity. ** indicates statutory RQ.
Sec.313: EPA SARA Title III Section 313 Toxic Release Inventory. Note: -Cat indicates a member of a chemical category.
Sec.110: EPA SARA 110 Superfund Site Priority Contaminant List

Other Important Lists:

CWA NPDES: EPA Clean Water Act NPDES Permit Chemical
CAA HAP: EPA Clean Air Act Hazardous Air Pollutant
CAA ODC: EPA Clean Air Act Ozone Depleting Chemical (1=CFC, 2=HCFC)
CA PROP 65: California Proposition 65

TSCA (Toxic Substances Control Act) Lists:

5A(2): Chemical Subject to Significant New Rules (SNURS)
6A: Commercial Chemical Control Rules
8A: Toxic Substances Subject To Information Rules on Production
8A CAIR: Comprehensive Assessment Information Rules - (CAIR)
8A PAIR: Preliminary Assessment Information Rules - (PAIR)
8C: Records of Allegations of Significant Adverse Reactions
8D: Health and Safety Data Reporting Rules
8D TERM: Health and Safety Data Reporting Rule Terminations

16. Other Information

Company Policy or Disclaimer

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