

# SAFETY DATA SHEET

Creation Date 16-Apr-2012

Revision Date 19-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

## 1. Identification

**Product Name** 2,2,6-Trimethyl-4H-1,3-dioxin-4-one

**Cat No. :** AC296910000; AC296910050; AC296911000; AC296915000

**CAS No** 5394-63-8  
**Synonyms** Diketene acetone adduct; TKD

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

### Details of the supplier of the safety data sheet

#### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

#### **Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## 2. Hazard(s) identification

### Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 2
Serious Eye Damage/Eye Irritation	Category 2

### Label Elements

#### **Signal Word**

Danger

#### **Hazard Statements**

Highly flammable liquid and vapor  
Causes serious eye irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
Keep container tightly closed  
Ground and bond container and receiving equipment  
Use explosion-proof electrical/ventilating/lighting equipment  
Wear protective gloves/protective clothing/eye protection/face protection  
Take action to prevent static discharges  
Use non-sparking tools

**Skin**

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
If eye irritation persists: Get medical advice/attention

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam to extinguish

**Storage**

Store in a well-ventilated place. Keep cool

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

None identified

**Hazards classified under paragraph (d)(1)(ii) of 1910.1200**

No information available

### 3. Composition/information on Ingredients

Component	CAS No	Weight %
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	> 93

### 4. First-aid measures

**General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water.

**Most important symptoms and effects**

. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

## Notes to Physician

Treat symptomatically

## 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray. Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Alcohol resistant foam. Water mist may be used to cool closed containers. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	14 °C / 57.2 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

**Specific Hazards Arising from the Chemical**

Vapors may form explosive mixture with air. Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

**Hazardous Combustion Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**NFPA**

**Health**  
2

**Flammability**  
3

**Instability**  
0

**Physical hazards**  
N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	Should not be released into the environment.
<b>Methods for Containment and Clean Up</b>	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 7. Handling and Storage

<b>Handling</b>	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.
<b>Storage.</b>	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame. Protect from light. Material darkens in color during storage. Do not allow contact with air. Incompatible Materials. Oxidizing agent.

## 8. Exposure controls / personal protection

<b>Exposure Guidelines</b>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
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**Engineering Measures** Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

#### Personal Protective Equipment

**Eye/face Protection** Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection** No protective equipment is needed under normal use conditions.

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

#### Appearance

#### **Physical State**

Liquid

#### **Color**

Dark brown

#### **Odor**

pungent

#### **Odor Threshold**

No information available

#### Property

#### Values

#### Remarks

#### • Method

#### **Melting Point/Range**

4 - 13 °C / 39.2 - 55.4 °F

#### **Softening Point**

No data available

#### **Boiling Point/Range**

65 - 67 °C / 149 - 152.6 °F

#### **Flash Point**

14 °C / 57.2 °F

#### **Flammability (liquid)**

Highly flammable

#### **Flammability (solid,gas)**

Not applicable

#### **Explosion Limits**

No data available

@ 2.7 MBAR

**Method** - No information available

On basis of test data

Liquid

#### **Autoignition Temperature**

No data available

#### **Decomposition Temperature**

&gt; 100°C

#### **pH**

No information available

#### **Viscosity**

No data available

#### **Water Solubility**

Insoluble

#### **Solubility in other solvents**

No information available

#### **Partition Coefficient (n-octanol/water)**

#### **Vapor Pressure**

No data available

#### **Density / Specific Gravity**

1.080

#### **Bulk Density**

Not applicable

Liquid

#### **Vapor Density**

4.9 (Air = 1.0)

(Air = 1.0)

#### **Particle characteristics**

Not applicable (liquid)

#### Other Information

#### **Molecular Formula**

C7 H10 O3

#### **Molecular Weight**

142.15

#### **Explosive Properties**

Vapors may form explosive mixtures with air

## 10. Stability and reactivity

**Reactive Hazard** None known, based on information available

<b>Stability</b>	Stable under normal conditions.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.
<b>Incompatible Materials</b>	Oxidizing agent
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> )
<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Information on expected route of exposure

<b>Inhalation</b>	Not an expected route of exposure.
<b>Ingestion</b>	May be harmful if swallowed.
<b>Eyes</b>	Avoid contact with eyes. Irritating to eyes. Lachrymator (substance which increases the flow of tears).
<b>Skin</b>	Avoid contact with skin. May cause irritation.

### Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	-	LD50 >= 5000 mg/kg ( Rabbit )	-

**Toxicologically Synergistic Products** No information available

**(b) skin corrosion/irritation;** No data available

**(c) serious eye damage/irritation;** Category 2

**(d) respiratory or skin sensitization;**  
**Respiratory** No data available  
**Skin** No data available

**(e) germ cell mutagenicity;** No data available

**(f) carcinogenicity;**

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	Not listed	Not listed	Not listed	Not listed	Not listed

**(g) reproductive toxicity;** No data available

**(h) STOT-single exposure;** No data available

**(i) STOT-repeated exposure;** No data available

<b>Target Organs</b>	No information available.
<b>(j) aspiration hazard;</b>	No data available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.
<b>Symptoms / effects, both acute and delayed</b>	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.
<b>Endocrine Disrupting Properties</b>	This product does not contain any known or suspected endocrine disruptors.

## 12. Ecological information

### Ecotoxicity

Do not empty into drains.

<b>Persistence and Degradability</b>	Persistence is unlikely based on information available.
<b>Bioaccumulation/ Accumulation</b>	No information available.
<b>Mobility</b>	Will likely be mobile in the environment due to its volatility.

## 13. Disposal considerations

<b>Waste Disposal Methods</b>	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
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## 14. Transport information

### DOT

<b>UN-No</b>	UN1993
<b>Proper Shipping Name</b>	Flammable liquid, n.o.s.
<b>Technical Shipping Name</b>	2,2,6-Trimethyl-4H-1,3-dioxin-4-one
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### TDG

<b>UN-No</b>	UN1993
<b>Proper Shipping Name</b>	Flammable liquid, n.o.s.
<b>Technical Shipping Name</b>	2,2,6-Trimethyl-4H-1,3-dioxin-4-one
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### IATA

<b>UN-No</b>	UN1993
<b>Proper Shipping Name</b>	Flammable liquid, n.o.s.
<b>Technical Shipping Name</b>	2,2,6-Trimethyl-4H-1,3-dioxin-4-one
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

### IMDG/IMO

<b>UN-No</b>	UN1993
<b>Proper Shipping Name</b>	Flammable liquid, n.o.s.
<b>Technical Shipping Name</b>	2,2,6-Trimethyl-4H-1,3-dioxin-4-one
<b>Hazard Class</b>	3
<b>Packing Group</b>	II

## 15. Regulatory Information

### United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	-	-	-

**Legend:**

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)**

Not applicable

**TSCA 12(b)** - Notices of Export

Not applicable

**International Inventories**

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	-	-	226-403-3	X	-		X	X	KE-34501

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)**U.S. Federal Regulations****SARA 313****SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)**

Not applicable

**Clean Air Act**

Not applicable

**OSHA** - Occupational Safety and Health Administration

Not applicable

**CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65**

This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations**

Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security**

This product does not contain any DHS chemicals.

**Other International Regulations****Mexico - Grade**

No information available

**Authorisation/Restrictions according to EU REACH**

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	-	-	-

**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	Not applicable	Not applicable	Not applicable	Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**

Not applicable

**Other International Regulations**

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
2,2,6-Trimethyl-4H-1,3-dioxin-4-one	5394-63-8	Not applicable	Not applicable	Not applicable	Not applicable

**16. Other Information****Prepared By**

Product stewardship (Regulatory Affairs)  
Thermo Fisher Scientific  
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**Creation Date**

16-Apr-2012

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**Revision Summary**

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text



**End of SDS**