Material Safety Data Sheet
2,2,6-Trimethyl-4H-1,3-dioxin-4-one, 90-95% (GC)

ACC# 97273

Section 1 - Chemical Product and Company Identification

MSDS Name: 2,2,6-Trimethyl-4H-1,3-dioxin-4-one, 90-95% (GC)
Catalog Numbers: AC296910000, AC296910050, AC296911000, NC9517604, NC9559165
Synonyms: Diketene acetone adduct.
Company Identification:
Fisher Scientific
1 Reagent Lane
Fair Lawn, NJ 07410
For information, call: 201-796-7100
Emergency Number: 201-796-7100
For CHEMTREC assistance, call: 800-424-9300
For International CHEMTREC assistance, call: 703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
5394-63-8	2,2,6-Trimethyl-1,3-dioxen-4-one	~90	226-403-3
67-64-1	Acetone	~4	200-662-2
141-79-7	4-Methyl-3-penten-2-one	<1	205-502-5
520-45-6	3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one	<1	208-293-9

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: orange to brown liquid. Flash Point: 14 deg C.
Warning! Flammable liquid and vapor. Causes eye irritation. May cause skin and respiratory tract irritation. May cause central nervous system depression. May cause kidney damage.
Target Organs: Kidneys, central nervous system.

Potential Health Effects
Eye: Causes eye irritation.
Skin: May cause skin irritation.
Ingestion: May cause irritation of the digestive tract. May cause kidney damage. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma and possible death due to respiratory failure.
Inhalation: Inhalation of high concentrations may cause central nervous system effects characterized by nausea, headache, dizziness, unconsciousness and coma. May cause respiratory tract irritation. May cause kidney damage.
Chronic: Prolonged or repeated skin contact may cause dermatitis. Chronic inhalation may cause effects similar to those of acute inhalation.

Section 4 - First Aid Measures

Eyes: Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid imme diately.
Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes.
Ingestion: If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately.
Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: Containers can build up pressure if exposed to heat and/or fire. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Use water spray to keep fire-exposed containers cool. Flammable liquid and vapor. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas. May be ignited by heat, sparks, and flame. Containers may explode when heated.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Cool containers with flooding quantities of water until well after fire is out.
Flash Point: 14 deg C (57.20 deg F)
Autoignition Temperature: Not available.
Explosion Limits, Lower:N/A

Upper: N/A
NFPA Rating: (estimated) Health: 1; Flammability: 3; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Clean up spills immediately, observing precautions in the Protective Equipment section. Remove all sources of ignition. Provide ventilation. A vapor suppressing foam may be used to reduce vapors. Water spray may reduce vapor but may not prevent ignition in closed spaces.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Use with adequate ventilation. Ground and bond containers when transferring material. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Avoid ingestion and inhalation. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
Storage: Keep away from heat, sparks, and flame. Keep away from sources of ignition. Keep container closed when not in use. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
2,2,6-Trimethyl-1,3-dioxen-4-one	none listed	none listed	none listed
Acetone	500 ppm TWA; 750 ppm STEL	250 ppm TWA; 590 mg/m3 TWA 2500 ppm IDLH	1000 ppm TWA; 2400 mg/m3 TWA
4-Methyl-3-penten-2-one	15 ppm TWA; 25 ppm STEL	10 ppm TWA; 40 mg/m3 TWA 1400 ppm IDLH	25 ppm TWA; 100 mg/m3 TWA
3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one	none listed	none listed	none listed

OSHA Vacated PELs: 2,2,6-Trimethyl-1,3-dioxen-4-one: No OSHA Vacated PELs are listed for this chemical. Acetone: 750 ppm TWA; 1800 mg/m3 TWA 4-Methyl-3-penten-2-one: 15 ppm TWA; 60 mg/m3 TWA 3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one: No OSHA Vacated PELs are listed for this chemical.
Personal Protective Equipment
Eyes: 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: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Liquid
Appearance: orange to brown
Odor: acetone-like
pH: Not available.
Vapor Pressure: Not available.
Vapor Density: 4.9
Evaporation Rate: Not available.
Viscosity: Not available.
Boiling Point: 65-67.0C
Freezing/Melting Point:4 deg C
Decomposition Temperature:> 100 deg C
Solubility: Insoluble.
Specific Gravity/Density:1.0880g/cm3
Molecular Formula:C7H10O3
Molecular Weight:142.15

Section 10 - Stability and Reactivity

Chemical Stability: Stable.
Conditions to Avoid: High temperatures, incompatible materials, ignition sources, excess heat, temperatures above 220°C, strong oxidants.
Incompatibilities with Other Materials: Acids (mineral, non-oxidizing, e.g. hydrochloric acid, hydrofluoric acid, muriatic acid, phosphoric acid), acids (mineral, oxidizing, e.g. chromic acid, hypochlorous acid, nitric acid, sulfuric acid), azo, diazo, and hydrazines (e.g. dimethyl hydrazine, hydrazine, methyl hydrazine), caustics (e.g. ammonia, ammonium hydrozide, calcium hydroxide, potassium hydroxide, sodium hydroxide), cyanides (e.g. potassium cyanide, sodium cyanide), mercaptans and other organic sulfides (e.g. butyl mercaptan, carbon disulfide, methanethiol), metals (alkali and alkaline, e.g. cesium, potassium, sodium), nitrides (e.g. potassium nitride, sodium nitride), peroxides and hydroperoxides (organic, e.g. acetyl peroxide, benzoyl peroxide, butyl peroxide, methyl ethyl ketone peroxide), oxidizing

agents (strong, e.g. bromine, hydrogen peroxide, nitrogen dioxide, potassium nitrate), reducing agents (strong, e.g. aluminum carbide, chlorosilane, hydrogen phosphide, lithium hydride), water reactive substances (e.g. acetic anyhdride, alkyl aluminum chloride, calcium carbide, ethyl dichlorosilane).
Hazardous Decomposition Products: Carbon monoxide, carbon dioxide.
Hazardous Polymerization: Has not been reported.

Section 11 - Toxicological Information

RTECS#:
CAS# 5394-63-8 unlisted.
CAS# 67-64-1: AL3150000
CAS# 141-79-7: SB4200000
CAS# 520-45-6: UP8050000
LD50/LC50:
Not available.

CAS# 67-64-1:
Dermal, guinea pig: LD50 = >9400 uL/kg;
Draize test, rabbit, eye: 20 mg Severe;
Draize test, rabbit, eye: 20 mg/24H Moderate;
Draize test, rabbit, eye: 10 uL Mild;
Draize test, rabbit, skin: 500 mg/24H Mild;
Inhalation, mouse: LC50 = 44 gm/m3/4H;
Inhalation, rat: LC50 = 50100 mg/m3/8H;
Oral, mouse: LD50 = 3 gm/kg;
Oral, rabbit: LD50 = 5340 mg/kg;
Oral, rat: LD50 = 5800 mg/kg;
.

CAS# 141-79-7:
Draize test, rabbit, eye: 20 mg Severe;
Inhalation, mouse: LC50 = 10 gm/m3/2H;
Inhalation, rat: LC50 = 9 gm/m3/4H;
Oral, mouse: LD50 = 710 mg/kg;
Oral, rabbit: LD50 = 1 gm/kg;
Oral, rat: LD50 = 1120 mg/kg;
Skin, rabbit: LD50 = 5150 mg/kg;
.

CAS# 520-45-6:
Oral, mouse: LD50 = 1330 mg/kg;
Oral, rat: LD50 = 500 mg/kg;
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Carcinogenicity:
CAS# 5394-63-8: Not listed by ACGIH, IARC, NTP, or CA Prop 65.
CAS# 67-64-1: Not listed by ACGIH, IARC, NTP, or CA Prop 65.
CAS# 141-79-7: Not listed by ACGIH, IARC, NTP, or CA Prop 65.
CAS# 520-45-6: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information available.
Teratogenicity: No information available.
Reproductive Effects: Fertility: post-implantation mortality. Ihl, mam: TCLo=31500 ug/m3/24H (1-13D preg)
Mutagenicity: Cytogenetic analysis: hamster fibroblast, 40 g/L Sex chromosome loss/non-disjunction: S.cerevisiae, 47600 ppm
Neurotoxicity: No information available.
Other Studies:

Section 12 - Ecological Information

Ecotoxicity: No data available. Rainbow trout LC50=5540 mg/L/96H Sunfish (tap water), death at 14250 ppm/24H Mosquito fish (turbid water) TLm=13000 ppm/48H
Environmental: Volatilizes, leeches, and biodegrades when released to soil.
Physical: No information available.
Other: None.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series:
CAS# 67-64-1: waste number U002 (Ignitable waste).

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	FLAMMABLE LIQUIDS, N.O.S.	FLAMMABLE LIQUID NOS (DIKETENE, ACETONE)

Hazard Class:	3	3
UN Number:	UN1993	UN1993
Packing Group:	II	II
Additional Info:		FP 14 C

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 5394-63-8 is not listed on the TSCA inventory. It is for research and development use only.
CAS# 67-64-1 is listed on the TSCA inventory.
CAS# 141-79-7 is listed on the TSCA inventory.
CAS# 520-45-6 is listed on the TSCA inventory.
Health & Safety Reporting List
CAS# 141-79-7: Effective 10/4/82, Sunset 10/4/92
Chemical Test Rules
CAS# 67-64-1: Test for Health Effects CAS# 141-79-7: Test for Health Effects
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
CAS# 67-64-1: 5000 lb final RQ; 2270 kg final RQ
SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.
SARA Codes
CAS # 67-64-1: immediate, fire.
CAS # 141-79-7: immediate, delayed, fire.
CAS # 520-45-6: immediate.
Section 313 No chemicals are reportable under Section 313.
Clean Air Act:
This material does not contain any hazardous air pollutants.
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.
Clean Water Act:
None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:
None of the chemicals in this product are considered highly hazardous by OSHA.
STATE
CAS# 5394-63-8 is not present on state lists from CA, PA, MN, MA, FL, or NJ.
CAS# 67-64-1 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.
CAS# 141-79-7 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.
CAS# 520-45-6 is not present on state lists from CA, PA, MN, MA, FL, or NJ.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives
Hazard Symbols:
F
Risk Phrases:
R 11 Highly flammable.

Safety Phrases:
S 16 Keep away from sources of ignition - No smoking.
S 26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
S 33 Take precautionary measures against static discharges.
S 36 Wear suitable protective clothing.
S 37 Wear suitable gloves.
S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
S 9 Keep container in a well-ventilated place.
S 28A After contact with skin, wash immediately with plenty of water
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WGK (Water Danger/Protection)
CAS# 5394-63-8: No information available.
CAS# 67-64-1: 0
CAS# 141-79-7: 1
CAS# 520-45-6: 1
Canada - DSL/NDSL
CAS# 67-64-1 is listed on Canada's DSL List.
CAS# 141-79-7 is listed on Canada's DSL List.
CAS# 520-45-6 is listed on Canada's DSL List.

Canada - WHMIS

This product has a WHMIS classification of B2, D2B.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

CAS# 67-64-1 is listed on the Canadian Ingredient Disclosure List.

CAS# 141-79-7 is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 7/08/1998
Revision #4 Date: 5/03/2005