

ALFAAA16248

4-Hydroxy-4-methyl-2-pentanone

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: 4-羟基-4-甲基-2-戊酮
Product Description: 4-Hydroxy-4-methyl-2-pentanone

Cat No. : A16248
Synonyms Diacetone alcohol
CAS No 123-42-2
Molecular Formula C6 H12 O2

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

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Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Clear

Odor
Pleasant

Emergency Overview

Flammable liquid and vapor. Causes serious eye irritation. May be harmful if swallowed. May cause respiratory irritation.
Suspected of damaging fertility or the unborn child.

Classification of the substance or mixture

Flammable liquids.	Category 3
Acute Oral Toxicity	Category 5
Serious Eye Damage/Eye Irritation	Category 2
Reproductive Toxicity	Category 2
Specific target organ toxicity - (single exposure)	Category 3

Label Elements

4-Hydroxy-4-methyl-2-pentanone

**Signal Word****Warning****Hazard Statements**

H226 - Flammable liquid and vapor
 H319 - Causes serious eye irritation
 H303 - May be harmful if swallowed
 H335 - May cause respiratory irritation
 H361 - Suspected of damaging fertility or the unborn child

Precautionary Statements**Prevention**

P201 - Obtain special instructions before use
 P202 - Do not handle until all safety precautions have been read and understood
 P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
 P240 - Ground and bond container and receiving equipment
 P241 - Use explosion-proof electrical/ ventilating/ lighting equipment
 P242 - Use non-sparking tools
 P243 - Take action to prevent static discharges
 P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
 P264 - Wash face, hands and any exposed skin thoroughly after handling
 P270 - Do not eat, drink or smoke when using this product
 P271 - Use only outdoors or in a well-ventilated area
 P280 - Wear eye protection/ face protection

Response

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell
 P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
 P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
 P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 P308 + P313 - IF exposed or concerned: Get medical advice/attention
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Vapors may cause flash fire or explosion. Flammable liquid.

Health Hazards

Causes serious eye irritation. May be harmful if swallowed. May cause respiratory irritation. Suspected of damaging fertility or the unborn child.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. . Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

Other Hazards

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Diacetone alcohol	123-42-2	>95

SECTION 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

None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Use personal protective equipment as required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

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

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

Should not be released into the environment.

Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

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Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Storage

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Component	China	Taiwan	Thailand	Hong Kong
Diacetone alcohol	TWA: 240 mg/m ³	TWA: 50 ppm TWA: 238 mg/m ³		-

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
Diacetone alcohol	TWA: 50 ppm	(Vacated) TWA: 50 ppm (Vacated) TWA: 240 mg/m ³ TWA: 50 ppm TWA: 240 mg/m ³	IDLH: 1800 ppm TWA: 50 ppm TWA: 240 mg/m ³	STEL: 75 ppm 15 min STEL: 362 mg/m ³ 15 min TWA: 50 ppm 8 hr TWA: 241 mg/m ³ 8 hr	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls**Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

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Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection	Long sleeved clothing
Respiratory Protection	In case of insufficient ventilation, wear suitable respiratory equipment. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly
Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387
Small scale/Laboratory use	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.
Environmental exposure controls	No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Clear	
Physical State	Liquid	
Odor	Pleasant	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-42.8 °C / -45 °F	
Softening Point	No data available	
Boiling Point/Range	166 °C / 330.8 °F	
Flash Point	58 °C / 136.4 °F	Method - No information available
Evaporation Rate	No information available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 1.8 Vol% Upper 6.9 Vol%	
Vapor Pressure	1 mmHg @ 20 °C	
Vapor Density	4.0 (Air = 1.0)	(Air = 1.0)
Specific Gravity / Density	0.939	
Bulk Density	Not applicable	Liquid
Water Solubility	Miscible	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Diacetone alcohol	1.03	
Autoignition Temperature	643 °C / 1189.4 °F	
Decomposition Temperature	No data available	
Viscosity	3.22 mPa.s @ 20°C	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C6 H12 O2	

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4-Hydroxy-4-methyl-2-pentanone

Molecular Weight 116.16

SECTION 10. STABILITY AND REACTIVITY

Stability Stable under normal conditions.

Hazardous Reactions None under normal processing.

Hazardous Polymerization Hazardous polymerization does not occur.

Conditions to Avoid Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

Materials to avoid Strong oxidizing agents. Alcohols. Amines. Acids. Strong bases.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Diacetone alcohol	LD50 > 4 g/kg (Rat)	LD50 = 13500 mg/kg (Rabbit) LD50 = 13630 mg/kg (Rabbit)	LC50 > 7.23 g/m ³ (Rat) 8 h

(b) skin corrosion/irritation; Based on available data, the classification criteria are not met

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory
Skin

Based on available data, the classification criteria are not met
Based on available data, the classification criteria are not met

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met
Not mutagenic in AMES Test

(f) carcinogenicity; Based on available data, the classification criteria are not met
There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Category 2

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

Target Organs None known.

(j) aspiration hazard; Based on available data, the classification criteria are not met

Symptoms / effects,both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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delayed

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Diacetone alcohol	LC50: = 420 mg/L, 96h (Lepomis macrochirus) LC50: = 420 mg/L, 96h static (Lepomis macrochirus)	EC50 = 8750 mg/L, 24h (Daphnia magna)		

Persistence and Degradability
Persistence Readily biodegradable
Persistence is unlikely.

Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Diacetone alcohol	1.03	No data available

Mobility in soil The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Highly mobile in soils.

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No UN1148
Proper Shipping Name DIACETONE ALCOHOL
Hazard Class 3
Packing Group III

IMDG/IMO

UN-No UN1148
Proper Shipping Name DIACETONE ALCOHOL
Hazard Class 3
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IATA

UN-No UN1148
Proper Shipping Name DIACETONE ALCOHOL
Hazard Class 3
Packing Group III

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION
International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Diacetone alcohol	X	X	X	X	204-626-7	X	X	X	X	X	X	X

National Regulations
SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 11-May-2010
Revision Date 26-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

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ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

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End of Safety Data Sheet