DIACETONE ALCOHOL (DAA)

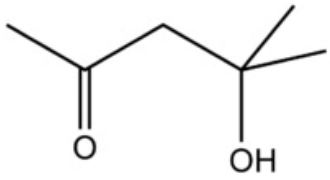
Chemical Formula: $C_6H_{12}O_2$

CAS Registry Number: 123-42-2

Molecular Weight: 116.16

Category: Alcohol

PRODUCT INFORMATION



Synonyms:

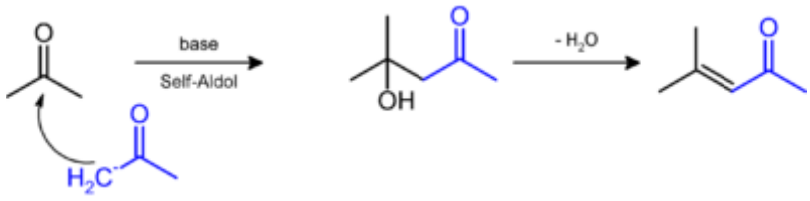
- 2-Hydroxy-2-methyl-4-pentanone
- 2-Methyl-2-pentanol-4-one
- 2-Methyl-4-oxo-2-pentanol
- 2-Pentanone, 4-hydroxy-4-methyl
- 2-Pentanone, 4-hydroxy-4-methyl-
- 4-hidroxi-4-metilpentan-2-ona
- 4-Hydroxy-2-keto-4-methylpentane
- 4-Hydroxy-4-methyl-2-oxopentane
- 4-Hydroxy-4-methyl-2-pentanone
- 4-Hydroxy-4-methylpentan-2-on
- 4-Hydroxy-4-methylpentan-2-one
- 4-hydroxy-4-methylpentane-2-one
- 4-Methyl-4-hydroxy-2-pentanone
- Acetonyldimethylcarbinol
- DIACETONALKOHOL
- DIACETONE ALCOHOL
- Diketone alcohol
- NSC 9005
- PENTAN-2-ONE, 4-HYDROXY-4-METHYL-
- Pyranton A
- Tyranton
- UN 1148

Diacetone alcohol is a chemical compound with the formula $CH_3C(O)CH_2C(OH)(CH_3)_2$. This liquid is a common synthetic intermediate used for the preparation of other compounds.

It is a natural ingredient of Sleepy grass (*Achnatherum robustum*).

Synthesis

First identified by Heintz, its preparation entails the $Ba(OH)_2$-catalyzed condensation of two molecules of acetone. It undergoes dehydration to give the α,β-unsaturated ketone, mesityl oxide:[3] Hydrogenation of mesityl oxide gives the industrial solvent, methyl isobutyl ketone("MIBK").



Physical and Chemical Properties

Appearance: Clear, colorless liquid.
Odor: Faint pleasant odor.
Solubility: Miscible in water.
Specific Gravity: 0.931 @ 25°C/4°C
pH: No information found.
% Volatiles by volume @ 21°C (70F): 100
Boiling Point: 172°C (342°F)
Melting Point: -44°C (-47°F)
Vapor Density (Air=1): 4.0
Vapor Pressure (mm Hg): 0.95 @ 20°C (68°F)
Evaporation Rate (BuAc=1): 0.14

Stability and Reactivity

Stability:
Stable under ordinary conditions of use and storage.
Hazardous Decomposition Products:
Carbon dioxide and carbon monoxide may form when heated to decomposition. May form acetone and mesityl oxide upon heating and by reaction with acids or bases.
Hazardous Polymerization:
Will not occur.
Incompatibilities:
Oxidizing agents, reducing agents, amines, alkanol, amines, aluminum, alkalis, pyridines, ammonia, isocyanates, inorganic acids and bases.
Conditions to Avoid:
Heat, flames, ignition sources and incompatibles. Note: Surfaces that are sufficiently hot may ignite diacetone alcohol, even in the absence of sparks and flame.

PT. Samchem Prasandha
Taman Palem Lestari Block A30 No. 26
Cengkareng - Jakarta 11730 - Indonesia
Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994

Hazards Identification

Emergency Overview

WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT. AFFECTS CENTRAL NERVOUS SYSTEM AND LIVER.

Health Rating: 2 - Moderate (Life)
Flammability Rating: 2 - Moderate
Reactivity Rating: 1 - Slight
Contact Rating: 3 - Severe
Lab Protective Equip: GOGGLES & SHIELD; LAB COAT & APRON; VENT HOOD; PROPER GLOVES; CLASS B EXTINGUISHER
Storage Color Code: Red (Flammable)

Potential Health Effects

Inhalation:
Causes irritation to the respiratory tract. Symptoms may include coughing, shortness of breath. Inhalation of high concentrations may affect the central nervous system and have a narcotic effect.
Ingestion:
Causes irritation to the gastrointestinal tract. Symptoms may include nausea, vomiting and diarrhea. Symptoms may parallel those from inhalation.
Skin Contact:
Causes skin irritation. May be absorbed through skin. May cause dermatitis.
Eye Contact:
Vapors cause eye irritation. Splashes cause severe irritation, possible corneal burns and eye damage.
Chronic Exposure:
Chronic exposure may affect kidneys and liver. Prolonged or repeated skin exposure may cause dermatitis.
Aggravation of Pre-existing Conditions:
Persons with pre-existing skin conditions or impaired respiratory function may be more susceptible to the effects of this substance.

First Aid Measures

Inhalation:
Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.
Ingestion:
Give large amounts of water to drink. Never give anything by mouth to an unconscious person. Get medical attention.
Skin Contact:
Immediately flush skin with plenty of soap and water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention if symptoms occur.
Eye Contact:
Immediately flush eyes with plenty of water for at least 15 minutes, lifting upper and lower eyelids occasionally. Get medical attention.

PT. Samchem Prasandha
Taman Palem Lestari Block A30 No. 26
Cengkareng - Jakarta 11730 - Indonesia
Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994

Fire Fighting Measures

Fire:
Flash point: 56°C (133°F) CC
Autoignition temperature: 603°C (1117°F)
Flammable limits in air % by volume:
lel: 1.8; uel: 6.9
Flammable Liquid and Vapor!
Note: Upon decomposition, diacetone alcohol may produce acetone or mesityl oxide which are more volatile and flammable than diacetone alcohol.
Explosion:
Above flash point, vapor-air mixtures are explosive within flammable limits noted above. Sealed containers may rupture when heated. Contact with strong oxidizers may cause fire. Sensitive to static discharge.
Fire Extinguishing Media:
Use alcohol foam, dry chemical or carbon dioxide. (Water may be ineffective.) Water spray may be used to keep fire exposed containers cool.
Special Information:
In the event of a fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus with full facepiece operated in the pressure demand or other positive pressure mode. Vapors can flow along surfaces to distant ignition source and flash back.

Accidental Release Measures

Ventilate area of leak or spill. Remove all sources of ignition. Wear appropriate personal protective equipment as specified in Section 8. Isolate hazard area. Keep unnecessary and unprotected personnel from entering. Contain and recover liquid when possible. Use non-sparking tools and equipment. Collect liquid in an appropriate container or absorb with an inert material (e. g., vermiculite, dry sand, earth), and place in a chemical waste container. Do not use combustible materials, such as saw dust. Do not flush to sewer! If a leak or spill has not ignited, use water spray to disperse the vapors, to protect personnel attempting to stop leak, and to flush spills away from exposures.

Handling and Storage

Protect against physical damage. Store in a cool, dry well-ventilated location, away from any area where the fire hazard may be acute. Outside or detached storage is preferred. Separate from incompatibles. Containers should be bonded and grounded for transfers to avoid static sparks. Storage and use areas should be No Smoking areas. Use non-sparking type tools and equipment, including explosion proof ventilation. Storage containers made from brass, bronze or lead may contaminate product. Containers of this material may be hazardous when empty since they retain product residues (vapors, liquid); observe all warnings and precautions listed for the product.

Exposure Controls/Personal Protection

Airborne Exposure Limits:
-OSHA Permissible Exposure Limit (PEL): 50 ppm (TWA)

PT. Samchem Prasandha
Taman Palem Lestari Block A30 No. 26
Cengkareng - Jakarta 11730 - Indonesia
Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994

-ACGIH Threshold Limit Value (TLV): 50 ppm (TWA)

Ventilation System:

A system of local and/or general exhaust is recommended to keep employee exposures below the Airborne Exposure Limits. Local exhaust ventilation is generally preferred because it can control the emissions of the contaminant at its source, preventing dispersion of it into the general work area. Please refer to the ACGIH document, *Industrial Ventilation, A Manual of Recommended Practices*, most recent edition, for details.

Personal Respirators (NIOSH Approved):

If the exposure limit is exceeded and engineering controls are not feasible, a full facepiece respirator with organic vapor cartridge may be worn up to 50 times the exposure limit or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. For emergencies or instances where the exposure levels are not known, use a full-facepiece positive-pressure, air-supplied respirator. WARNING: Air purifying respirators do not protect workers in oxygen-deficient atmospheres.

Skin Protection:

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

Eye Protection:

Use chemical safety goggles and/or a full face shield where splashing is possible. Maintain eye wash fountain and quick-drench facilities in work area.

Ecological Information

Environmental Fate:

When released into the soil, this material may biodegrade to a moderate extent. When released into the soil, this material may leach into groundwater. When released into the soil, this material may evaporate to a moderate extent. When released into water, this material may biodegrade to a moderate extent. When released into water, this material is not expected to evaporate significantly. This material has a log octanol-water partition coefficient of less than 3.0. This material is not expected to significantly bioaccumulate. When released into the air, this material is expected to be readily degraded by reaction with photochemically produced hydroxyl radicals. When released into the air, this material may be moderately degraded by photolysis. When released into the air, this material may be removed from the atmosphere to a moderate extent by wet deposition. When released into air, this material is expected to have a half-life between 10 and 30 days.

Environmental Toxicity:

This material is not expected to be toxic to aquatic life. The LC50/96-hour values for fish are over 100 mg/l.

Other Information

NFPA Ratings: Health: **1** Flammability: **2** Reactivity: **0**

Label Hazard Warning:

WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT. AFFECTS CENTRAL NERVOUS SYSTEM AND LIVER.

Label Precautions:

Avoid breathing vapor.
Avoid contact with eyes, skin and clothing.
Keep container closed.
Use only with adequate ventilation.
Wash thoroughly after handling.
Keep away from heat, sparks and flame.

PT. Samchem Prasandha
Taman Palem Lestari Block A30 No. 26
Cengkareng - Jakarta 11730 - Indonesia
Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994

Label First Aid:
In case of contact, immediately flush eyes or skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. If swallowed, give large amounts of water to drink. Never give anything by mouth to an unconscious person. In all cases, get medical attention.

Applications

Diacetone alcohol has slow evaporation rates. It is used as a solvent for both hydrogen bonding and polar substances. It is miscible in water and used as a solvent for water-based coatings. It is used as a solvent extractant in purification processes for resins and waxes. Diacetone alcohol is more suitable for use in applications as a component of gravure printing inks, with proving favorable flow and leveling characteristics. Diacetone alcohol, having hydroxyl and carbonyl group in the same molecule is used as a chemical intermediate.

PT. Samchem Prasandha
Taman Palem Lestari Block A30 No. 26
Cengkareng - Jakarta 11730 - Indonesia
Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994