



Safety Data Sheet

1. PRODUCT IDENTIFICATION

| | |
|--------------|--|
| Name | Diacetone Alcohol |
| Synonyms | 4-hydroxy-4-methyl-2-pentanone; 4-hydroxy-4-methylpentan-2-one; 4-hydroxy-2-keto-4-methylpentane |
| CAS# | 123-42-2 |
| Europe EC# | 204-626-7 |
| Product Uses | organic synthesis, cellulose solvent, coatings solvent & others |

2. HAZARDS

Quick Guide: combustible liquid; irritating to eyes; vapour irritating to eyes & respiratory system

Canada – WHMIS

Key:

B 3, D 2B

B 2 – Flash Point <38°C, B 3 – Flash Point >38°C & <93°C

D 1 – Immediately Toxic, D 2 – Chronic Toxicity

C – Oxidising Substance, E – Corrosive, F – Reactive Substance



B3 – Combustible Liquid

U.S.A. – HMIS

Key:

Health – 2, Fire – 2, Reactivity – 0

0=minimal, 1=slight, 2=moderate, 3=serious, 4=severe



D2B – Toxic

3. COMPOSITION

| | % | TWAEV / TLV mg/m ³ | LD ₅₀ (mg/kg) ORAL | LD ₅₀ (mg/kg) SKIN | LC ₅₀ ppm INHALATION |
|--------------------------------|------|----------------------------------|----------------------------------|----------------------------------|------------------------------------|
| 4-hydroxy-4-methyl-2-pentanone | 100% | 50 / 240 | 2520 | 13,500 | 1860 |

4. FIRST AID

| | |
|-------------|---|
| SKIN: | Wash with plenty of water. Remove contaminated clothing and do not reuse until thoroughly laundered. |
| EYES: | Wash eyes with plenty of water, holding eyelids open. Seek medical assistance promptly if there is irritation. |
| INHALATION: | Remove from contaminated area promptly. CAUTION: Rescuer must not endanger himself! If breathing stops, administer artificial respiration and seek medical aid promptly. |
| INGESTION: | Give plenty of water to dilute product. Do not induce vomiting (NOTE below). Keep victim quiet. If vomiting occurs, lower victim's head below hips to prevent inhalation of vomited material. Seek medical help promptly. |

Inadvertent inhalation of vomited material may seriously damage the lungs. The danger of this is greater than the risk of poisoning through absorption of this relatively low-toxicity substance. The stomach should only be emptied under medical supervision, and after the installation of an airway to protect the lungs.

5. FIRE FIGHTING & FLAMMABILITY

| | |
|----------------------------|---|
| Flash Point | 64°C / 148°F (closed cup) – <i>assumes the product is essentially acetone-free; see Part 14</i> |
| Autoignition Temperature | 603°C / 1118°F – <i>643°C/1190°F for commercial grade containing some acetone</i> |
| Flammable Limits | 1.8% – 6.9% |
| Combustion Products | carbon monoxide, nitrogen oxides, smoke, part oxidised hydrocarbon fragments |
| Firefighting Precautions | foam, dry chemical, water fog or spray, product floats on water – water jet spreads flames; firefighters must wear SCBA |
| Static Charge Accumulation | cannot accumulate a static charge on agitation or pumping |

Please ensure that this MSDS is given to, and explained to people using this product.

6. ACCIDENTAL RELEASE MEASURES

Leak Precaution dyke to control spillage and prevent environmental contamination
 Handling Spill ventilate contaminated area; recover free liquid with suitable pumps; absorb residue on an inert sorbent, sweep,
 shovel & store in closed containers for recycling or disposal

7. HANDLING & STORAGE

Store in a cool, dry environment, away from sources of ignition, heat and oxidising agents. Empty containers may contain a flammable / explosive vapour (*of acetone*). Always ensure that containers, whether empty or full, or part full, are tightly sealed unless in use. *If prolonged storage is anticipated, maintain product in a slightly alkaline state to prevent decomposition.*

Avoid breathing product vapour. Use with adequate ventilation if product mist is created. If dealing with a spill, and ventilation is impossible or impractical, wear a suitable respirator with organic vapour cartridge.

Never cut, drill, weld or grind on or near this container. Avoid contact with skin and wash work clothes frequently. An eye bath and safety shower must be available near the workplace.

8. EXPOSURE CONTROL & PERSONAL PROTECTION

| | | | |
|----------------|--|--------------|------------------------------|
| Ontario TWA/EV | 50ppm / 240mg/m ³ | Ontario STEV | 75ppm / 360mg/m ³ |
| ACGIH TLV | 50ppm / 238mg/m ³ | | |
| OSHA PEL | 50ppm / 240mg/m ³ | | |
| Ventilation | mechanical ventilation may be required to control airborne titre | | |
| Hands | wear butyl rubber or "Barrier" gloves – <i>other types also protect; consult supplier to confirm suitability</i> | | |
| Eyes | safety glasses with side shields – <i>always protect the eyes</i> | | |
| Clothing | no special protective clothing required | | |

9. PHYSICAL PROPERTIES

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|---|---|
| Odour & Appearance | clear, colourless liquid with "dusty" faintly minty odour; <i>yellowes on prolonged storage</i> |
| Odour Threshold | ~1ppm |
| Vapour Pressure | 1mmHg / 0.13kPa (20°C / 68°F) |
| Evaporation Rate (<i>Butyl Acetate = 1</i>) | 0.1 |
| Vapour Density (air = 1) | 4 |
| Boiling Range | 168°C / 334°F |
| Freezing Point | -44°C / -47°F |
| Specific Gravity | 0.94 (20/20°C) |
| Water Solubility | complete |
| Also soluble in | most organic solvents |
| Viscosity | 2.9centipoise (25°C / 77°F) |
| pH | none – (<i>does not liberate hydrogen ions when dissolved</i>) |
| Conversion Factor | 1ppm = 4.74mg/m ³ |
| Molecular Weight | 116grams per mole |

10. REACTIVITY

| | |
|--------------------------------|-----------------------------|
| Dangerously Reactive With | strong oxidising agents |
| Also Reactive With | strong alkalis |
| Stability | stable; will not polymerize |
| Decomposes in Presence of | acidic conditions |
| Decomposition Products | acetone |
| Sensitive to Mechanical Impact | no |

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11. TOXICITY

Effects, Acute Exposure

| | |
|-----------------|---|
| Skin Contact | moderately irritating; skin redness likely if contact is prolonged |
| Skin Absorption | slight; no toxic effects likely by this route |
| Eye Contact | irritating liquid; vapour irritating at 100ppm; eye damage seen in test animals |
| Inhalation | vapour irritating at 100ppm (20 min); 2100ppm causes restlessness and sleepiness in animals |
| Ingestion | not known – <i>not a route of industrial exposure</i> |

Effects, Chronic Exposure

| | |
|-------------------------------|--|
| General | prolonged exposure may cause dermatitis; liver and kidney damage may occur; destruction of red blood cells has been seen in test animals |
| Sensitising | not a sensitiser in humans or animals |
| Carcinogen/Tumorigen | not considered a tumorigen or a carcinogen in humans or animals |
| Reproductive Effect | no known effect in humans or animals |
| Mutagen | no known effect on humans or animals |
| Synergistic With | not known |
| LD ₅₀ (oral) | 2520 & 4000mg/kg (rat), 3000 & 3950mg/kg (mouse), 4653mg/kg (rabbit), |
| LD ₅₀ (skin) | 13,630mg/kg (rabbit) |
| LC ₅₀ (inhalation) | >1500 & >1860ppm (rat) – <i>no mortality in either test</i> |

12. ECOLOGICAL INFORMATION

| | |
|------------------------------------|---|
| Bioaccumulation | not a bioaccumulator |
| Biodegradation | biodegrades readily & rapidly in the presence of oxygen; 31-47% in 5 days; 100% in 14 days |
| Abiotic Degradation | reacts with atmospheric hydroxyl radicals; estimated ½-life in air is 12 days |
| Mobility in soil, water | water soluble: moves readily in soil & water – <i>if biodegradation does not destroy it first</i> |
| Aquatic Toxicity | |
| LC ₅₀ (Fish, 96hr) | 420mg/litre (Lepomis macrochirus & Menidia berylinia) |
| EC ₅₀ (Crustacea, 24hr) | 9000mg/litre (Daphnia magna) |
| EC ₅₀ (Algae) | 530mg/litre (Microcystis aeruginosa) |
| EC ₃ (Algae) | 3000mg/litre (Scenedesmus quadricauda) – <i>this is an EC₃, not an EC₅₀</i> |
| EC ₃ (Bacteria) | 825mg/litre (Pseudomonas putida) – <i>this is an EC₃, not an EC₅₀</i> |

13. DISPOSAL

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|----------------|---|
| Waste Disposal | do not flush to sewer , recycle solvent if possible, may be incinerated in approved facility |
| Containers | Drums should be reused. Recondition and pressure test by a licensed reconditioner prior to re-use. Pails must be vented and thoroughly dried prior to crushing and recycling. IBCs (intermediate bulk containers): polyethylene bottle must be pressure tested & recertified at 30 months. Replace at 60 months (5yrs). Steel containers must be inspected, pressure tested & recertified every 5 years. <i>Never cut, drill, weld or grind on or near this container, even if empty</i> |

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14. TRANSPORT CLASSIFICATION

| | | |
|------------------|-----------------------|------------------------|
| Canada TDG | PIN | UN - 1148 |
| AND | Shipping Name | diacetone alcohol |
| U.S.A. 49 CFR | Class & Packing Group | 3 (III)* |
| Marine Pollutant | | not a marine pollutant |
| ERAP Required | | NO |



* NOTE: If the product is impure (with above 2-3% acetone) the Packing Group changes to II.

EMERGENCY INFORMATION

| | | |
|--------|------------------------|----------------|
| Canada | Call CANUTEC (collect) | (613) 996-6666 |
| U.S.A. | Call CHEMTREC | (800) 424-9300 |

15. REGULATIONS

| | |
|---------------|--------------|
| Canada DSL | on inventory |
| U.S.A. TSCA | on inventory |
| Europe EINECS | on inventory |

Europe Classification



| | |
|-----------------------|---|
| Europe Risk Phrases | R: 36 – Irritating to eyes. |
| Europe Safety Phrases | S: 24/25 – Avoid contact with skin or eyes. |

Immediately Dangerous to Life or Health: 1800 ppm

Allowable Tolerances: Diacetone alcohol is exempted from the requirement of a tolerance when used as a deactivator or a solvent for formulations used before crop emerges from soil in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

OSHA Standards: Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 50 ppm (240 mg/cu m).

NIOSH Recommendations: Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 50 ppm (240 mg/cu m).

Threshold Limit Values: 8 hr Time Weighted Avg (TWA): 50 ppm. Excursion Limit Recommendation: Excursions in worker exposure levels may exceed three times the TLV-TWA for no more than a total of 30 min during a work day, and under no circumstances should they exceed five times the TLV-TWA, provided that the TLV-TWA is not exceeded.

Atmospheric Standards: This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to use the best demonstrated system of continuous emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. Diacetone alcohol is produced, as an intermediate or final product, by process units covered under this subpart.

FIFRA Requirements: Diacetone alcohol is exempted from the requirement of a tolerance when used as a deactivator or a solvent for formulations used before crop emerges from the soil in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

FDA Requirements: Diacetone alcohol is an indirect food additive for use only as a component of adhesives.

16. OTHER INFORMATION

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Data from RTECS, HSDB (Haz. Substance Data Base), Cheminfo (CCOHS), IUCLID Datasheets (ESIS – European Chem. Substance Info. System), & others.

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