

SAFETY DATA SHEET

Version 6.5
Revision Date 10/07/2021
Print Date 11/13/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : Acetoin
Product Number : W200808
Brand : Aldrich
CAS-No. : 513-86-0**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +1 314 771-5765
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Flammable liquids (Category 3), H226
Serious eye damage (Category 1), H318

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)
H226 : Flammable liquid and vapor.
H318 : Causes serious eye damage.

Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 3-Hydroxy-2-butanone
Acetylmethylcarbinol

Formula : C₄H₈O₂
Molecular weight : 88.11 g/mol
CAS-No. : 513-86-0
EC-No. : 208-174-1

Component	Classification	Concentration
Acetoin		
	Flam. Liq. 3; Eye Dam. 1; H226, H318	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures**5.1 Extinguishing media****Suitable extinguishing media**

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage stability

Recommended storage temperature
2 - 8 °C

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 90 °C (194 °F)
f) Initial boiling point and boiling range	148 °C 298 °F - lit.
g) Flash point	ca.48 °C (118 °F) at ca.1013 hPa - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 12.2 %(V) Lower explosion limit: 1 %(V)
k) Vapor pressure	ca.8.6 hPa at ca.20 °C (ca.68 °F)
l) Vapor density	No data available
m) Density	1.013 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	soluble
o) Partition coefficient: n-octanol/water	Pow: ca.0.1 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	367 °C (693 °F) at 1005.0 hPa
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Strong oxidizing agents, Strong bases

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - > 2,000 mg/kg
(OECD Test Guideline 423)

Inhalation: No data available

LD50 Dermal - Rabbit - > 5,000 mg/kg
No data available

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE)

Result: No skin irritation
(OECD Test Guideline 439)

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

Direct Peptide Reactivity Assay (DPRA)

Result: Not a skin sensitizer.
(OECD Test Guideline 442C)

Germ cell mutagenicity

Test Type: reverse mutation assay

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

- NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: EL8790000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish LC50 - Leuciscus idus (Golden orfe) - > 2,200 mg/l - 96 h

LC0 - Leuciscus idus (Golden orfe) - 2,200 mg/l - 48 h

Toxicity to bacteria

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: ca.76 % - Readily biodegradable.
(OECD Test Guideline 301F)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information**DOT (US)**

UN number: 2621 Class: 3 Packing group: III
Proper shipping name: Acetyl methyl carbinol
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2621 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: ACETYL METHYL CARBINOL

IATA

UN number: 2621 Class: 3 Packing group: III
Proper shipping name: Acetyl methyl carbinol

SECTION 15: Regulatory information**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

Acetoin, dimer	CAS-No. 513-86-0	Revision Date 2007-03-01
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New Jersey Right To Know Components

Acetoin, dimer	CAS-No. 513-86-0	Revision Date 2007-03-01
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SECTION 16: Other information

Further information

December 23, 2009, the USA Center of Disease Control-NIOSH in a letter updating USA Department of Labor-OSHA, stated it is planning to conduct research of three diacetyl substitutes; (1) starter mix, a distillate that contains diacetyl; (2) acetoin, prepared from diacetyl and used for its butter-like odor; and (3) 2,3pentanedione, a constituent of butter flavoring agents which NIOSH described as "structurally very similar to diacetyl." Exposure to diacetyl may cause nausea, headache, and vomiting.

For additional studies related to this product, review OSHA literature on Diacetyl and flavorings (www.OSHA.gov), the OSHA NEP for Microwave Popcorn Processing Plants, NIOSH publication 2004-110d, and other NIOSH literature regarding flavorings (www.cdc.gov/NIOSH).

Animals exposed to diacetyl and other related diacetyl substitutes experienced damage to the nose and upper airways, including severe damage to cells lining the respiratory tract. NIOSH has reported that employees exposed to butter flavorings containing diacetyl are at risk of developing occupational lung diseases and that in one instance, similar illnesses have been found among employees producing butter and vanilla flavorings containing diacetyl.

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