

SAFETY DATA SHEET

Version 6.11
Revision Date 08/05/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Acetoin

Product Number : W200832

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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +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 Statements

H226

Flammable liquid and vapor.

H318

Causes serious eye damage.

Precautionary Statements

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

No data available

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

No data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Combustible.

5.3 Advice for firefighters

No data available

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

6.2 Environmental precautions

No data available

6.3 Methods and materials for containment and cleaning up

No data available

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

No data available

7.3 Specific end use(s)

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

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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

No data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: liquid
Color: colorless, to, light yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: 15 °C (59 °F)
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 |

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- 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

No data available

10.2 Chemical stability

No data available

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

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

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Carcinogenicity

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.

Reproductive toxicity

Specific target organ toxicity - single exposure

Specific target organ toxicity - repeated exposure

Aspiration hazard

11.2 Additional Information

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

SECTION 12: Ecological information

12.1 Toxicity

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

No data available

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

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Acute Health Hazard

SARA 313

: 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations**Massachusetts Right To Know**

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

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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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