

## SAFETY DATA SHEET

Version 6.0  
Revision Date 08/07/2019  
Print Date 06/01/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 4-Methyl-2-pentanone-1,1,1,3,3-d<sub>5</sub>

Product Number : 487724  
Brand : Aldrich  
CAS-No. : 4840-81-7

**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 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 number**

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 2), H225  
Acute toxicity, Inhalation (Category 4), H332  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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)        |                                                                                                                                  |
| H225                       | Highly flammable liquid and vapour.                                                                                              |
| H319                       | Causes serious eye irritation.                                                                                                   |
| H332                       | Harmful if inhaled.                                                                                                              |
| H335                       | May cause respiratory irritation.                                                                                                |
| 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.                                                                            |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.                                                                           |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P271                       | Use only outdoors or in a well-ventilated area.                                                                                  |
| 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.                              |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.       |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                                             |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                                                 |
| P403 + P235                | Store in a well-ventilated place. Keep cool.                                                                                     |
| P405                       | Store locked up.                                                                                                                 |
| 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 : Deuterated 4-methyl-2-pentanone  
Isopropylacetone-D5  
Deuterated methyl isobutyl ketone

Formula : C<sub>6</sub>D<sub>5</sub>H<sub>7</sub>O  
Molecular weight : 105.15 g/mol  
CAS-No. : 4840-81-7

| Component                                | Classification                                                                     | Concentration |
|------------------------------------------|------------------------------------------------------------------------------------|---------------|
| <b>4-Methyl-2-pentanone-1,1,1,3,3-d5</b> |                                                                                    |               |
|                                          | Flam. Liq. 2; Acute Tox. 4;<br>Eye Irrit. 2A; STOT SE 3;<br>H225, H332, H319, H335 | <= 100 %      |

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## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Dry powder Dry sand

#### Unsuitable extinguishing media

Do NOT use water jet.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas.

Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

## **6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## **6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

## **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

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

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### **Personal protective equipment**

##### **Eye/face protection**

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

##### **Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

|                                                 |                                                                      |
|-------------------------------------------------|----------------------------------------------------------------------|
| a) Appearance                                   | Form: liquid                                                         |
| b) Odour                                        | No data available                                                    |
| c) Odour Threshold                              | No data available                                                    |
| d) pH                                           | No data available                                                    |
| e) Melting point/freezing point                 | Melting point/range: -80 °C (-112 °F)                                |
| f) Initial boiling point and boiling range      | 117 - 118 °C 243 - 244 °F - lit.                                     |
| g) Flash point                                  | 14.00 °C (57.20 °F) - 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: 8.00 %(V)<br>Lower explosion limit: 1.20 %(V) |
| k) Vapour pressure                              | 20 hPa at 20.00 °C (68.00 °F)                                        |
| l) Vapour density                               | No data available                                                    |
| m) Relative density                             | 0.841 g/mL at 25 °C (77 °F)0.841 g/cm <sup>3</sup> at 25 °C (77 °F)  |
| n) Water solubility                             | No data available                                                    |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.310                                                       |
| p) Auto-ignition temperature                    | No data available                                                    |
| q) Decomposition temperature                    | No data available                                                    |
| r) Viscosity                                    | No data available                                                    |
| s) Explosive properties                         | No data available                                                    |

t) Oxidizing properties No data available

## **9.2 Other safety information**

No data available

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## **SECTION 10: Stability and reactivity**

### **10.1 Reactivity**

No data available

### **10.2 Chemical stability**

Stable under recommended storage conditions.

### **10.3 Possibility of hazardous reactions**

Vapours may form explosive mixture with air.

### **10.4 Conditions to avoid**

Heat, flames and sparks.

### **10.5 Incompatible materials**

Oxidizing agents, Strong bases

### **10.6 Hazardous decomposition products**

No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

LD50 Oral - Rat - 2,080 mg/kg

LC50 Inhalation - Rat - 4.00 h - 8.2 - 16.4 mg/l

LD50 Dermal - Rabbit - > 16,000 mg/kg

No data available

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: Mild skin irritation - 24.00 h

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Moderate eye irritation - 24.00 h

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No component 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 component 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

No data available

**Specific target organ toxicity - single exposure**

May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

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

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish LC0 - Leuciscus idus melanotus - 480 mg/l - 48.0 h

**12.2 Persistence and degradability**

No data available

**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 Other adverse effects**

No data available

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**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1245    Class: 3    Packing group: II  
Proper shipping name: Methyl isobutyl ketone  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1245    Class: 3    Packing group: II    EMS-No: F-E, S-D  
Proper shipping name: METHYL ISOBUTYL KETONE

### IATA

UN number: 1245    Class: 3    Packing group: II  
Proper shipping name: Methyl isobutyl ketone

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## SECTION 15: Regulatory information

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### 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

|                                   |                      |               |
|-----------------------------------|----------------------|---------------|
| 4-Methyl-2-pentanone-1,1,1,3,3-d5 | CAS-No.<br>4840-81-7 | Revision Date |
|-----------------------------------|----------------------|---------------|

|                                   |                      |               |
|-----------------------------------|----------------------|---------------|
| 4-Methyl-2-pentanone-1,1,1,3,3-d5 | CAS-No.<br>4840-81-7 | Revision Date |
|-----------------------------------|----------------------|---------------|

### New Jersey Right To Know Components

|                                   |                      |               |
|-----------------------------------|----------------------|---------------|
| 4-Methyl-2-pentanone-1,1,1,3,3-d5 | CAS-No.<br>4840-81-7 | Revision Date |
|-----------------------------------|----------------------|---------------|

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## SECTION 16: Other information

### Further information

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