

Creation Date 05-Sep-2014

Revision Date 29-Sep-2023

Revision Number 5

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

**Product Description:** Acetylacetaldehyde dimethyl acetal  
**Cat No. :** 292330000; 292330010; 292330050; 292332500  
**Synonyms** KBA; 3-Ketobutyraldehyde dimethyl acetal; 3-Oxobutyraldehyde dimethylacetal; 4,4-Dimethoxy-2-butanone  
**CAS No** 5436-21-5  
**Molecular Formula** C6 H12 O3

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### 1.3. Details of the supplier of the safety data sheet

#### Company

**UK entity/business name**  
 Fisher Scientific UK  
 Bishop Meadow Road,  
 Loughborough, Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
 Thermo Fisher Scientific  
 Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

**E-mail address** begel.sdsdesk@thermofisher.com

### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Flammable liquids

Category 3 (H226)

##### Health hazards

Based on available data, the classification criteria are not met

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## **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



**Signal Word**

**Warning**

## **Hazard Statements**

H226 - Flammable liquid and vapor

## **Precautionary Statements**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

| Component                  | CAS No    | EC No             | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567 |
|----------------------------|-----------|-------------------|----------|---|
| 2-Butanone, 4,4-dimethoxy- | 5436-21-5 | EEC No. 226-605-1 | 95       | Flam. Liq. 3 (H226)   |

Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

### **4.1. Description of first aid measures**

#### **Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

#### **Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.

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|                                    |  |
|------------------------------------|--|
| Ingestion                          | Do NOT induce vomiting. Get medical attention.   |
| Inhalation                         | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.                       |
| Self-Protection of the First Aider | Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination. |

## 4.2. Most important symptoms and effects, both acute and delayed

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

## 4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

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

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

Remove all sources of ignition. Take precautionary measures against static discharges.

### 6.2. Environmental precautions

See Section 12 for additional Ecological Information.

### 6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not let this chemical enter the environment.

### 6.4. Reference to other sections

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Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid contact with skin and eyes. Avoid contact with skin and clothing. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges.

### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 3  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

#### **Predicted No Effect Concentration (PNEC)**

No information available.

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## 8.2. Exposure controls

### Engineering Measures

Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

#### Hand Protection

Protective gloves

| Glove material                                      | Breakthrough time                 | Glove thickness | EU standard | Glove comments        |
|---|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber<br>Neoprene<br>Natural rubber<br>PVC | See manufacturers recommendations | -               | EN 374      | (minimum requirement) |

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

#### Respiratory Protection

No protective equipment is needed under normal use conditions.

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

#### Small scale/Laboratory use

Maintain adequate ventilation

#### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

|                           |                          |                                   |
|---------------------------|--------------------------|-----------------------------------|
| Physical State            | Liquid                   |                                   |
| Appearance                | Clear                    |                                   |
| Odor                      | No information available |                                   |
| Odor Threshold            | No data available        |                                   |
| Melting Point/Range       | -82 °C / -115.6 °F       |                                   |
| Softening Point           | No data available        |                                   |
| Boiling Point/Range       | 178 °C / 352.4 °F        |                                   |
| Flammability (liquid)     | Flammable                | On basis of test data             |
| Flammability (solid,gas)  | Not applicable           | Liquid                            |
| Explosion Limits          | No data available        |                                   |
| Flash Point               | 49 °C / 120.2 °F         | Method - No information available |
| Autoignition Temperature  | 285 °C / 545 °F          |                                   |
| Decomposition Temperature | No data available        |                                   |
| pH                        | 3.5                      | 10 g/L aq.sol                     |
| Viscosity                 | 1.503 mPa s at 20 °C     |                                   |

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|   |                          |             |
|---|--------------------------|-------------|
| Water Solubility                        | decomposes               |             |
| Solubility in other solvents            | No information available |             |
| Partition Coefficient (n-octanol/water) |                          |             |
| Vapor Pressure                          | 1 hPa @ 20 °C            |             |
| Density / Specific Gravity              | 0.990                    |             |
| Bulk Density                            | Not applicable           | Liquid      |
| Vapor Density                           | 4.56                     | (Air = 1.0) |
| Particle characteristics                | Not applicable (liquid)  |             |

## 9.2. Other information

|                      |  |
|----------------------|--|
| Molecular Formula    | C6 H12 O3                              |
| Molecular Weight     | 132.16                                 |
| Explosive Properties | explosive air/vapour mixtures possible |

## SECTION 10: STABILITY AND REACTIVITY

|                         |  |
|-------------------------|--|
| <u>10.1. Reactivity</u> | None known, based on information available |
|-------------------------|--|

|                                 |                                 |
|---------------------------------|---------------------------------|
| <u>10.2. Chemical stability</u> | Stable under normal conditions. |
|---------------------------------|---------------------------------|

### 10.3. Possibility of hazardous reactions

|                          |                           |
|--------------------------|---------------------------|
| Hazardous Polymerization | No information available. |
| Hazardous Reactions      | No information available. |

|                                  |   |
|----------------------------------|---|
| <u>10.4. Conditions to avoid</u> | Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.<br>Exposure to moisture. |
|----------------------------------|---|

|                                     |                                 |
|-------------------------------------|---------------------------------|
| <u>10.5. Incompatible materials</u> | Acids. Strong oxidizing agents. |
|-------------------------------------|---------------------------------|

|   |  |
|---|--|
| <u>10.6. Hazardous decomposition products</u> | Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). |
|---|--|

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

|                     |  |
|---------------------|--|
| (a) acute toxicity; |  |
| Oral                | Based on available data, the classification criteria are not met |
| Dermal              | No data available  |
| Inhalation          | No data available  |

| Component                  | LD50 Oral                 | LD50 Dermal | LC50 Inhalation |
|----------------------------|---------------------------|-------------|-----------------|
| 2-Butanone, 4,4-dimethoxy- | LD50 = 6200 mg/kg ( Rat ) | -           | -               |

|                                |                   |
|--------------------------------|-------------------|
| (b) skin corrosion/irritation; | No data available |
|--------------------------------|-------------------|

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(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available

Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

Ecotoxicity effects Do not empty into drains.

### 12.2. Persistence and degradability

Persistence Soluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

12.4. Mobility in soil The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB No data available for assessment.

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## assessment

### 12.6. Endocrine disrupting properties

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

### 12.7. Other adverse effects

**Persistent Organic Pollutant** This product does not contain any known or suspected substance

**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Waste from Residues/Unused Products** Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

**European Waste Catalogue (EWC)** According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

**Other Information** Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

**14.1. UN number** UN1993  
**14.2. UN proper shipping name** Flammable liquid, n.o.s.  
**Technical Shipping Name** (ACETYLACETALDEHYDE DIMETHYL ACETAL)  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III

### ADR

**14.1. UN number** UN1993  
**14.2. UN proper shipping name** Flammable liquid, n.o.s.  
**Technical Shipping Name** (ACETYLACETALDEHYDE DIMETHYL ACETAL)  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III

### IATA

**14.1. UN number** UN1993  
**14.2. UN proper shipping name** Flammable liquid, n.o.s.  
**Technical Shipping Name** (ACETYLACETALDEHYDE DIMETHYL ACETAL)  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III



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- 14.5. Environmental hazards** No hazards identified
- 14.6. Special precautions for user** No special precautions required.
- 14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component                  | CAS No    | EINECS    | ELINCS | NLP | IECSC | TCSI | KECL     | ENCS | ISHL |
|----------------------------|-----------|-----------|--------|-----|-------|------|----------|------|------|
| 2-Butanone, 4,4-dimethoxy- | 5436-21-5 | 226-605-1 | -      | -   | -     | X    | KE-11047 | X    | X    |

| Component                  | CAS No    | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|----------------------------|-----------|------|---|-----|------|------|-------|-------|
| 2-Butanone, 4,4-dimethoxy- | 5436-21-5 | X    | ACTIVE  | X   | -    | X    | X     | X     |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

#### Authorisation/Restrictions according to EU REACH

Not applicable

| Component                  | CAS No    | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|----------------------------|-----------|---|---|---|
| 2-Butanone, 4,4-dimethoxy- | 5436-21-5 | -   | -   | -   |

#### Seveso III Directive (2012/18/EC)

| Component                  | CAS No    | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|----------------------------|-----------|---|--|
| 2-Butanone, 4,4-dimethoxy- | 5436-21-5 | Not applicable  | Not applicable   |

#### Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

#### Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

#### National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

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## WGK Classification

Water endangering class = 2 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H226 - Flammable liquid and vapor

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer  
Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

### Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Creation Date** 05-Sep-2014

**Revision Date** 29-Sep-2023

**Revision Summary** Not applicable.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

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## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**