

# SAFETY DATA SHEET

Version 6.9  
Revision Date 03/02/2024  
Print Date 06/15/2024

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Acetone-d<sub>6</sub>

Product Number : 444863  
Brand : Aldrich  
CAS-No. : 666-52-4

### 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 2), H225  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

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

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## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225

Highly flammable liquid and vapor.

H319

Causes serious eye irritation.

H336

May cause drowsiness or dizziness.

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.

P261

Avoid breathing mist or vapors.

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

Repeated exposure may cause skin dryness or cracking.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Hexadeuteroacetone

Formula : C<sub>3</sub>D<sub>6</sub>O

Molecular weight : 64.12 g/mol

CAS-No. : 666-52-4

EC-No. : 211-563-9

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Component	Classification	Concentration
<b>(2H6)acetone</b>		
	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336	<= 100 %

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

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## 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. Call in physician.

#### 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. 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO2) Foam 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.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.  
Forms explosive mixtures with air at ambient temperatures.

### **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.

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## **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.

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

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

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **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. Preventive skin protection recommended. 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.

Store under inert gas. hygroscopic

#### **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

Component	CAS-No.	Value	Control parameters	Basis
(2H6)acetone	666-52-4	TWA	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		
		TWA	250 ppm 590 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	1,000 ppm 2,400 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	3,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	500 ppm 1,200 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	750 ppm 1,780 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
(2H6)acetone	666-52-4	Acetone	25 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. 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). Safety glasses

### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Latex gloves

Minimum layer thickness: 0.6 mm

Break through time: 10 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

### Body Protection

Flame retardant antistatic protective clothing.

### Respiratory protection

Recommended Filter type: Filter type AX

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |                   |
|-------------------|-------------------|
| a) Appearance     | Form: liquid      |
| b) Odor           | No data available |
| c) Odor Threshold | No data available |

d) pH	No data available
e) Melting point/freezing point	Melting point/range: -93.8 °C (-136.8 °F) - lit.
f) Initial boiling point and boiling range	55.5 °C 131.9 °F - lit.
g) Flash point	-19 °C (-2 °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: 13.2 %(V) Lower explosion limit: 2.15 %(V)
k) Vapor pressure	245 hPa at 20 °C (68 °F)
l) Vapor density	2.21 - (Air = 1.0)
m) Density	0.872 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
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

Relative vapor density	2.21 - (Air = 1.0)
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Risk of explosion with:  
chromosulfuric acid

chromyl chloride  
ethanolamine  
Fluorine  
Strong oxidizing agents  
strong reducing agents  
Nitric acid  
chromium(VI) oxide  
nonmetallic oxyhalides  
halogen-halogen compounds  
Chloroform  
nitrating acid  
nitrosyl compounds  
hydrogen peroxide  
halogen oxides  
organic nitro compounds  
peroxi compounds  
Risk of ignition or formation of inflammable gases or vapours with:  
Exothermic reaction with:  
Bromine  
Alkali metals  
alkali hydroxides  
Halogenated hydrocarbon  
Sulfur dichloride  
phosphorous oxichloride

#### **10.4 Conditions to avoid**

Avoid moisture.  
Warming.

#### **10.5 Incompatible materials**

No data available

#### **10.6 Hazardous decomposition products**

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 - female - 5,800 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: acetone

Symptoms: Stomach/intestinal disorders, Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.

LC50 Inhalation - Rat - 4 h - 76 mg/l - vapor

Remarks: Unconsciousness

Drowsiness

Dizziness

(External MSDS)

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The value is given in analogy to the following substances: acetone  
LD50 Dermal - Rabbit - 20,000 mg/kg

Remarks: (IUCLID)

The value is given in analogy to the following substances: acetone

### **Skin corrosion/irritation**

Skin - Rabbit

Result: Mild skin irritation - 24 h

(Draize Test)

Remarks: (RTECS)

The value is given in analogy to the following substances: acetone

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

Eyes - Rabbit

Result: Eye irritation - 24 h

(Draize Test)

Remarks: (RTECS)

The value is given in analogy to the following substances: acetone

### **Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: acetone

Chronic exposure may cause dermatitis.

### **Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: acetone  
Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: acetone  
Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances:

### **acetone 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**

Inhalation - May cause drowsiness or dizziness. - Narcotic effects

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: acetone

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

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

After absorption:

Headache

Salivation

Nausea

Vomiting

Dizziness

narcosis

Coma

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Kidney - Irregularities - Based on Human Evidence

Skin - Dermatitis - Based on Human Evidence

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**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish                      flow-through test LC50 - Pimephales promelas (fathead minnow) -  
6,210 mg/l - 96 h  
(OECD Test Guideline 203)  
Remarks: The value is given in analogy to the following substances:  
acetone

Toxicity to daphnia                      static test LC50 - Daphnia pulex (Water flea) - 8,800 mg/l - 48 h  
and other aquatic                      Remarks: (ECHA)  
invertebrates                      The value is given in analogy to the following substances: acetone

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Toxicity to algae	static test NOEC - M.aeruginosa - 530 mg/l - 8 d (DIN 38412) Remarks: (maximum permissible toxic concentration) (IUCLID) The value is given in analogy to the following substances: acetone
Toxicity to bacteria	static test EC50 - activated sludge - 61.15 mg/l - 30 min (OECD Test Guideline 209) Remarks: The value is given in analogy to the following substances: acetone
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - Daphnia magna (Water flea) - 2,212 mg/l - 28 d Remarks: (ECHA) The value is given in analogy to the following substances: acetone

## 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 91 % - Readily biodegradable. (OECD Test Guideline 301B) Remarks: The value is given in analogy to the following substances: acetone
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## 12.3 Bioaccumulative potential

Does not bioaccumulate.

## 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

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**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.

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

UN number: 1090 Class: 3 Packing group: II  
Proper shipping name: Acetone  
Reportable Quantity (RQ): 5000 lbs  
Reportable Quantity (RQ): 100 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1090 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: ACETONE

**IATA**

UN number: 1090 Class: 3 Packing group: II  
Proper shipping name: Acetone

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**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, Chronic Health Hazard

**Reportable Quantity** : F003 lbs

**Massachusetts Right To Know Components**

(2H6)acetone	CAS-No. 666-52-4	Revision Date 1993-02-16
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**Pennsylvania Right To Know Components**

(2H6)acetone	CAS-No. 666-52-4	Revision Date 1993-02-16
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## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.

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