

## SAFETY DATA SHEET

Version 6.3  
Revision Date 15.04.2022  
Print Date 03.06.2022**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

**1.3 Details of the supplier of the safety data sheet**Company : MilliporeSigma Canada Ltd  
2149 WINSTON PARK DRIVE  
OAKVILLE ON L6H 6J8  
CANADATelephone : +1 905 829-9500  
Fax : +1 905 829-9292**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 Hazardous Products Regulations (HPR) (SOR/2015-17)**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.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal Word

Danger

Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
Precautionary statement(s)	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharges.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
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.

- none

## 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

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

Aldrich - 444863

Page 2 of 10

	H336	
* Weight %		

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. 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

---

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

---

### 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 safe handling

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

Contains no substances with occupational exposure limit values.

### 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

##### 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   |
| 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)<br>Lower explosion limit: 2.15 %(V) |
| k) Vapor pressure                               | 245 hPa at 20 °C (68 °F)   |
| l) Vapor density                                | 2.21 - (Air = 1.0)   |

Aldrich - 444863

Page 5 of 10

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)
---------------------------	--------------------

---

## 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:

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:

Activated charcoal

chromosulfuric acid

chromyl chloride

ethanolamine

Fluorine

Strong oxidizing agents

strong reducing agents

Nitric acid

chromium(VI) oxide

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

rubber, various plastics

#### 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 - 5,800 mg/kg

Remarks: (ECHA)

(in analogy to similar products)

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

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

Remarks: Unconsciousness

Drowsiness

Dizziness

(External MSDS)

(in analogy to similar products)

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

LD50 Dermal - Rabbit - 20,000 mg/kg

Remarks: (IUCLID)

(in analogy to similar products)

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

No data available

##### Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 24 h

(Draize Test)

Remarks: (RTECS)

(in analogy to similar products)

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)

(in analogy to similar products)

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

##### Respiratory or skin sensitization

No data available

### **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: (in analogy to similar products)

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: (in analogy to similar products)

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: (in analogy to similar products)

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

**Carcinogenicity**  
No data available

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

May cause drowsiness or dizziness.

Remarks: (in analogy to similar products)

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.

Stomach - Irregularities - Based on Human Evidence

---

## **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: (in analogy to similar products) The value is given in analogy to the following substances: acetone
------------------	---

Toxicity to daphnia and other aquatic	static test LC50 - Daphnia pulex (Water flea) - 8,800 mg/l - 48 h Remarks: (ECHA)
---------------------------------------	--

Aldrich - 444863

Page 8 of 10

invertebrates	(in analogy to similar products) The value is given in analogy to the following substances: acetone
Toxicity to algae	static test NOEC - M.aeruginosa - 530 mg/l - 8 d (DIN 38412) Remarks: (maximum permissible toxic concentration) (in analogy to similar products) 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: (in analogy to similar products) The value is given in analogy to the following substances: acetone

## 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 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](http://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

### TDG

UN number: 1090    Class: 3    Packing group: II  
 Proper shipping name: ACETONE  
 Labels: 3  
 ERG Code: 127  
 Marine pollutant: no

### IMDG

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

Aldrich - 444863

Page 9 of 10

Proper shipping name: ACETONE

**IATA**

UN number: 1090 Class: 3

Packing group: II

Proper shipping name: Acetone

---

**SECTION 15: Regulatory information**

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

---

**SECTION 16: Other information**

**Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.3

Revision Date: 15.04.2022

Print Date: 03.06.2022