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

1.1 Product identifiers

- Product name: Acetone-d₆
- Product Number: 151793
- 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: 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.

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/ 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.

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2H6)acetone</td>
<td>Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Synonyms: Hexadeuteroacetone
Formula: C₃D₆O
Molecular weight: 64.12 g/mol
CAS-No.: 666-52-4
EC-No.: 211-563-9
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 (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.
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
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 Information

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2H6)acetone</td>
<td>666-52-4</td>
<td>TWA 250 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
<td>Remarks Not classifiable as a human carcinogen</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 500 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
<td>Not classifiable as a human carcinogen</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA 250 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>590 mg/m³</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>C 3000 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL 500 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1200 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 750 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1780 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
</tbody>
</table>

### Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2H6)acetone</td>
<td>666-52-4</td>
<td>Acetone</td>
<td>25 mg/l</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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**  
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

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: liquid</td>
</tr>
<tr>
<td>b) Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: -93.8 °C (-136.8 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>55.5 °C 131.9 °F - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>-19 °C (-2 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 13.2 %(V)</td>
</tr>
<tr>
<td></td>
<td>Lower explosion limit: 2.15 %(V)</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>245 hPa at 20 °C (68 °F)</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>2.21 - (Air = 1.0)</td>
</tr>
</tbody>
</table>
m) Density
   Relative density: 0.872 g/cm³ at 25 °C (77 °F) - lit.

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
   - peroxy 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:
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

**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**
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

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 invertebrates
static test LC50 - Daphnia pulex (Water flea) - 8,800 mg/l - 48 h
Remarks: (ECHA)
(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

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)
(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.

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
Proper shipping name: ACETONE

EMS-No: F-E, S-D

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

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

Pennsylvania Right To Know Components

Aldrich - 151793
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 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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