SAFETY DATA SHEET

Version 8.6
Revision Date 05/17/2025
Print Date 05/18/2025

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Acetone-d_6

Product Number : 434523
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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids : Category 2

Eye irritation : Category 2A

Specific target organ toxicity - single exposure	:	Category 3 (Central nervous system)

Other hazards

Repeated exposure may cause skin dryness or cracking.

GHS label elements

Hazard pictograms :

Signal Word : Danger

Hazard Statements : H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.

Precautionary statements :

Prevention:

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.

Response:

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.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(2H6)acetone	666-52-4*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this 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.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing : Carbon dioxide (CO2)

media		Foam Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Pay attention to flashback. Vapours 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.
Hazardous combustion products	:	Carbon oxides
Specific extinguishing methods	:	No data available
Further information	:	Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, 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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains. Risk of explosion.
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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on storage conditions	:	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.
Storage class	:	3, Flammable liquids
Recommended storage temperature	:	Recommended storage temperature see product label.
Further information on storage stability	:	Store under inert gas. hygroscopic
Packaging material	:	Suitable material: Clear Glass Ampules

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type:	:	Filter type AX

The entrepeneur 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.

Hand protection

Material	:	butyl-rubber
Break through time	:	480 min
Glove thickness	:	0.3 mm
Protective index	:	Full contact
Manufacturer	:	Butoject® (KCL 897 / Aldrich Z677647, Size M)

Material	:	butyl-rubber
Break through time	:	480 min
Glove thickness	:	0.3 mm
Protective index	:	Splash contact
Manufacturer	:	Butoject® (KCL 897 / Aldrich Z677647, Size M)

Manufacturer	:	data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
Remarks	:	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. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards

such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection	:	Flame retardant antistatic protective clothing.
Hygiene measures	:	Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid
Color	:	No data available
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	-136.8 °F / -93.8 °C Method: lit.
Boiling point/boiling range	:	131.9 °F / 55.5 °C Method: lit.
Flash point	:	-2 °F / -19 °C Method: closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	13.2 %(V)
Lower explosion limit / Lower flammability limit	:	2.15 %(V)
Vapor pressure	:	245 hPa (68 °F / 20 °C)
Relative vapour density	:	2.21 (Air = 1.0)
Relative density	:	No data available

Density	:	0.872 g/cm3 (77 °F / 25 °C) Method: lit.
Water solubility	:	No data available
Partition coefficient: n-octanol/water	:	No data available
Autoignition temperature	:	869 °F / 465 °C DIN 51794
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	No data available
Molecular weight	:	64.12 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapours may form explosive mixture with air.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
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
Sulphur dichloride
phosphorous oxichloride

Conditions to avoid	:	Avoid moisture. Warming.
Incompatible materials	:	rubber various plastics
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)
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 - vapour

Remarks: Unconsciousness
Drowsiness
Dizziness
(External MSDS)
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
Maximisation 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: acetoneTest 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: acetoneTest 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 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

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

(2H6)acetone:

Toxicity to fish	:	LC50 (Pimephales promelas (fathead minnow)): 6,210 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 203 Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: acetone
Toxicity to daphnia and other aquatic invertebrates	:	LC50 (Daphnia pulex (Water flea)): 8,800 mg/l End point: mortality Exposure time: 48 h Test Type: static test

Remarks: (ECHA)
The value is given in analogy to the following substances:
The value is given in analogy to the following substances: acetone

Toxicity to algae/aquatic plants : NOEC (M.aeruginosa): 530 mg/l
Exposure time: 8 d
Test Type: static test
Method: DIN 38412
Remarks: (maximum permissible toxic concentration) (IUCLID)
The value is given in analogy to the following substances:
The value is given in analogy to the following substances: acetone

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 2,212 mg/l
End point: reproduction rate
Exposure time: 28 d
Test Type: flow-through test
Remarks: (ECHA)
The value is given in analogy to the following substances:
The value is given in analogy to the following substances: acetone

Toxicity to microorganisms : EC50 (activated sludge): 61.15 mg/l
Exposure time: 30 min
Test Type: static test
Method: OECD Test Guideline 209
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: acetone

Persistence and degradability

Components:

(2H6)acetone:

Biodegradability : aerobic
Inoculum: activated sludge
Result: Readily biodegradable.
Biodegradation: 91 %
Exposure time: 28 d
Method: OECD Test Guideline 301B
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: acetone

Bioaccumulative potential

Components:

(2H6)acetone:

Bioaccumulation	:	Bioconcentration factor (BCF): < 10 Remarks: Does not bioaccumulate.

Mobility in soil

No data available

Other adverse effects

Components:

(2H6)acetone:

Results of PBT and vPvB assessment	:	Substance is not persistent, bioaccumulative, and toxic (PBT). Substance is not very persistent and very bioaccumulative (vPvB).
	:	Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	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

International Regulations

IATA-DGR

UN/ID No.	:	UN 1090
Proper shipping name	:	Acetone
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	364
Packing instruction (passenger aircraft)	:	353

IMDG-Code

UN number	:	UN 1090
Proper shipping name	:	ACETONE

Class	:	3
Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-D
Marine pollutant	:	no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number	:	UN 1090
Proper shipping name	:	Acetone
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
ERG Code	:	127
Marine pollutant	:	no
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards	:	Fire Hazard Acute Health Hazard Chronic Health Hazard
SARA 313	:	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.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Massachusetts Right To Know

(2H6)acetone	666-52-4

Pennsylvania Right To Know

(2H6)acetone	666-52-4

Pennsylvania Right To Know

(2H6)acetone	666-52-4

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

New Jersey Right To Know

(2H6)acetone	666-52-4

The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a

test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Details in analogy to the undeuterated compound.

Revision Date : 05/17/2025

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