



MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 12/12/2012

Version 1.2

SECTION 1. Identification

Product identifier

Product number	100021
Millipore Ref.	1000210010 ACETONE-D6 DEUTERATION DEGREE MIN. 99.8%
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™

Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Use restricted under TSCA to research and development or as analytical reagent. Uses regulated under FDA or FIFRA are not affected. Reagent for analysis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America SDS Phone Support: +1-978-715-1335 General Inquiries: +1-978-751-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 2, H225
Specific target organ systemic toxicity - single exposure, Category 3, H336
Eye irritation, Category 2, H319
For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms



Signal Word

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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.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P403 + P235 Store in a well-ventilated place. Keep cool.

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	CD ₃ COCD ₃	C ₃ D ₆ O (Hill)
CAS-No.	666-52-4	
Molar mass	64.12 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

(2H6)acetone (<= 100 %)

666-52-4

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Consult doctor if feeling unwell.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing.

Eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

Ingestion

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Drowsiness, Dizziness, narcosis, Nausea, Vomiting, Stomach/intestinal disorders, Headache, drowsiness, Salivation, Coma

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Risk of corneal clouding.

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

Development of hazardous combustion gases or vapors possible in the event of fire.

Advice for firefighters

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Cool closed containers exposed to fire with water spray.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into drains. Explosive properties

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. Chemisorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

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

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Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Conditions for safe storage, including any incompatibilities

Protected from light. Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>(2H6)acetone 666-52-4</i>			
ACGIH	Time Weighted Average (TWA):	500 ppm	
	Short Term Exposure Limit (STEL):	750 ppm	
NIOSH/GUIDE	Recommended exposure limit (REL):	250 ppm 590 mg/m ³	
OSHA_TRANS	PEL:	1,000 ppm 2,400 mg/m ³	
Z1A	Time Weighted Average (TWA):	750 ppm 1,800 mg/m ³	
	Short Term Exposure Limit (STEL):	1,000 ppm 2,400 mg/m ³	

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

Flame retardant antistatic protective clothing

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Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	characteristic
Odor Threshold	200 - 400 ppm
pH	5 - 6 at 365 g/l
Melting point	-139.7 °F (-95.4 °C)
Boiling point/boiling range	133.2 °F (56.2 °C) at 1,013 hPa
Flash point	< -4 °F (< -20 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	2.6 %(V)
Upper explosion limit	12.8 %(V)
Vapor pressure	233 hPa at 68 °F (20 °C)
Relative vapor density	No information available.
Relative density	0.88 g/cm ³ at 68 °F (20 °C)
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: -0.24 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).

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Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0.32 mPa.s at 68 °F (20 °C)
Explosive properties	Not classified as explosive.
Ignition temperature	869 °F (465 °C) DIN 51794

SECTION 10. Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

Sensitivity to light

Possibility of hazardous reactions

Risk of explosion with:

nonmetallic oxyhalides, halogen-halogen compounds, Chloroform, nitrating acid, nitrosyl compounds, hydrogen peroxide

Risk of ignition or formation of flammable gases or vapors 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

Conditions to avoid

Warming.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Incompatible materials

rubber, various plastics

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Target Organs

Eyes

Skin

Respiratory system

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Central nervous system

Acute oral toxicity

LD50 rat: 5,800 mg/kg (RTECS)

Symptoms: Stomach/intestinal disorders, Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

absorption

Acute inhalation toxicity

LC50 rat: 76 mg/l; 4 h (Lit.)

Symptoms: mucosal irritations

absorption

Acute dermal toxicity

LD50 rabbit: 20,000 mg/kg

(IUCLID)

slow absorption

Skin irritation

rabbit

Result: No irritation

(External MSDS)

Repeated exposure may cause skin dryness or cracking.

Eye irritation

rabbit

Result: Eye irritation

(External MSDS)

Risk of corneal clouding.

Causes serious eye irritation.

Sensitization

Sensitization test: guinea pig

Result: negative

(Lit.)

Genotoxicity in vivo

Mutagenicity (mammal cell test): micronucleus.

Result: negative

(National Toxicology Program)

Genotoxicity in vitro

Ames test

Result: negative

(National Toxicology Program)

Mutagenicity (mammal cell test): chromosome aberration.

Result: negative

(National Toxicology Program)

Carcinogenicity

Did not show carcinogenic effects in animal experiments. (IUCLID)

Specific target organ systemic toxicity - single exposure

May cause drowsiness or dizziness.

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Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
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.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

After absorption:

Headache, Salivation, Nausea, Vomiting, Dizziness, narcosis, Coma

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 *Oncorhynchus mykiss* (rainbow trout): 5,540 mg/l; 96 h (Lit.)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia magna* (Water flea): 6,100 mg/l; 48 h (Lit.)

EC5 *E.sulcatum*: 28 mg/l; 72 h (Lit.)

Toxicity to algae

IC5 *Scenedesmus quadricauda* (Green algae): 7,500 mg/l; 8 d (IUCLID)

IC5 *M.aeruginosa*: 530 mg/l; 8 d (IUCLID)

Toxicity to bacteria

EC5 *Pseudomonas putida*: 1,700 mg/l; 16 h (maximum permissible toxic concentration) (IUCLID)

Persistence and degradability

Biodegradability

91 %; 28 d

(IUCLID)

Readily biodegradable.

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Biochemical Oxygen Demand (BOD)

1,850 mg/g (5 d)
(IUCLID)

Chemical Oxygen Demand (COD)

2,070 mg/g
(IUCLID)

Theoretical oxygen demand (ThOD)

2,200 mg/g
(Lit.)

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -0.24
(experimental)

(Lit.) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 1090
Proper shipping name	ACETONE
Class	3
Packing group	II
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 1090
Proper shipping name	ACETONE
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

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UN number	UN 1090
Proper shipping name	ACETONE
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-E S-D

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Flammable Liquid
Eye irritant
Target organ effects

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard
Acute Health Hazard
Chronic Health Hazard

US State Regulations

Massachusetts Right To Know

Ingredients
(2H6)acetone

Pennsylvania Right To Know

Ingredients
(2H6)acetone

New Jersey Right To Know

Ingredients
(2H6)acetone

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.

DSL: This product contains one or several components that are not on the Canadian DSL nor NDSL.

SECTION 16. Other information

Details in analogy to the undeuterated compound.

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Training advice

Provide adequate information, instruction and training for operators.

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

H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Revision Date 12/12/2012

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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