

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 25.04.2017

Version 14.11

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

1.1 Product identifier

Catalogue No.	100021
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	666-52-4

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

Identified uses	Reagent for analysis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225

Specific target organ 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.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.

H319 Causes serious eye irritation.

H336 May cause drowsiness or dizziness.

EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

Response

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

Storage

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 100021
Product name Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy
MagniSolv™

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

CAS-No. 666-52-4

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CD ₃ COCD ₃	C ₃ D ₆ O (Hill)
EC-No.	211-563-9	
Molar mass	64,12 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
(2H6)acetone (≤ 100 %)		
666-52-4	*)	

Flammable liquid, Category 2, H225

Eye irritation, Category 2, H319

Specific target organ toxicity - single exposure, Category 3, H336

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

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3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Dizziness, narcosis, Nausea, Vomiting, Stomach/intestinal disorders, Headache, Salivation, Coma

Risk of corneal clouding.

irritant effects, somnolence, Drowsiness, Repeated exposure may cause skin dryness or cracking.

4.3 Indication of any immediate medical attention and special treatment needed

No information 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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™

Combustible.

Vapours 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 vapours possible in the event of fire.

5.3 Advice for firefighters

Special protective equipment for firefighters

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

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system. Suppress (knock down) gases/vapours/mists with a water spray jet. Cool closed containers exposed to fire with water spray.

SECTION 6. Accidental release measures

6.1 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:

Protective equipment 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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

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.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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

Recommended storage temperature see product label.

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

8.2 Exposure controls

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Engineering measures

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

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	natural latex
Glove thickness:	0,6 mm
Break through time:	> 10 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 706 Lapren® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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).

Other protective equipment

Flame retardant antistatic protective clothing.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter AX (EN 371)

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.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	characteristic
Odour Threshold	200 - 400 ppm
pH	5 - 6 at 365 g/l
Melting point	-95,4 °C
Boiling point/boiling range	56,2 °C at 1.013 hPa
Flash point	< -20 °C Method: c.c.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Evaporation rate	No information available.
Flammability (solid, gas)	Not applicable
Lower explosion limit	2,6 %(V)
Upper explosion limit	12,8 %(V)
Vapour pressure	233 hPa at 20 °C
Relative vapour density	No information available.
Density	0,88 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: -0,24 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0,32 mPa.s at 20 °C
Explosive properties	Not classified as explosive.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Oxidizing properties	none
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9.2 Other data

Ignition temperature	465 °C DIN 51794
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SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

Sensitivity to light

Sensitive to air.

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, Sulphur dichloride, phosphorous oxichloride

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 5.800 mg/kg

(RTECS)

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

Acute inhalation toxicity

LC50 Rat: 76 mg/l; 4 h ; vapour

(Lit.)

Symptoms: Possible symptoms:, mucosal irritations

Acute dermal toxicity

LD50 Rabbit: 20.000 mg/kg

(IUCLID)

Skin irritation

Rabbit

Result: No irritation

(External MSDS)

Repeated exposure may cause skin dryness or cracking.

Eye irritation

Rabbit

Result: Eye irritation

(External MSDS)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Risk of corneal clouding.

Causes serious eye irritation.

Sensitisation

Sensitisation test: Guinea pig

Result: negative

(Lit.)

Germ cell mutagenicity

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)

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

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.

SECTION 12. Ecological information

12.1 Toxicity

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)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
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12.2 Persistence and degradability

Biodegradability

91 %; 28 d

(IUCLID)

Readily biodegradable

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.)

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -0,24

(experimental)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	100021
Product name	Acetone-D6 deuteration degree min. 99.9% for NMR spectroscopy MagniSolv™

SECTION 13. Disposal considerations

Waste treatment methods

See 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

Land transport (ADR/RID)

14.1 UN number	UN 1090
14.2 Proper shipping name	ACETONE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1090
14.2 Proper shipping name	ACETONE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

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

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard	SEVESO III
Legislation	FLAMMABLE LIQUIDS P5c Quantity 1: 5.000 t Quantity 2: 50.000 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 3

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Details in analogy to the undeuterated compound.

Details in analogy to the undeuterated compound.

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

H225 Highly flammable liquid and vapour.

H319 Causes serious eye irritation.

H336 May cause drowsiness or dizziness.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

SAFETY DATA SHEET

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Danger

Hazard statements

H225 Highly flammable liquid and vapour.

H319 Causes serious eye irritation.

H336 May cause drowsiness or dizziness.

EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240 Ground/bond container and receiving equipment.

Response

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

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.