

according to Regulation (EC) No. 1907/2006

Revision Date 17.11.2017

Version 3.6

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

1.1 Product identifier

Catalogue No. 113366

Product name Deuterium oxide 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. 7789-20-0

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

Identified uses Reagent for development and research

For additional information on uses please refer to the Merck Chemicals

portal (www.merckgroup.com).

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 Please contact the regional company representation in your country.

number

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

This substance is not classified as dangerous according to European Union legislation.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula D₂O (Hill)

EC-No. 232-148-9

Molar mass 20,03 g/mol

Remarks No disclosure requirement according to Regulation (EC) No.

1907/2006.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

After inhalation: fresh air.

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.

No special precautionary measures necessary.

4.2 Most important symptoms and effects, both acute and delayed

We have no description of any toxic symptoms.

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

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Not combustible.

5.3 Advice for firefighters

Special protective equipment for firefighters

none

Further information

none

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

none

6.2 Environmental precautions

No special precautionary measures necessary.

6.3 Methods and materials for containment and cleaning up

Pour into drain.

Observe possible material restrictions (see sections 7 and 10).

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.

Hygiene measures

not required

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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.

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

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

not required

Hand protection

not required

Respiratory protection

not required

Environmental exposure controls

No special precautionary measures necessary.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

Form liquid

Colour colourless

Odour odourless

Odour Threshold Not applicable

pH ca. 7

at 20 °C

Melting point 3,8 °C

Boiling point/boiling range 101 °C

at 1.013 hPa

Flash point does not flash

Evaporation rate No information available.

Flammability (solid, gas) No information available.

Lower explosion limit not combustible

Upper explosion limit not combustible

Vapour pressure No information available.

Relative vapour density No information available.

Density 1,11 g/cm3

at 20 °C

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

Relative density No information available.

Water solubility at 20 °C

soluble

Partition coefficient: n-

octanol/water Not applicable

Auto-ignition temperature does not ignite

Decomposition temperature No information available.

Viscosity, dynamic No information available.

Explosive properties Not applicable

Oxidizing properties none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

See section 10.3

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

The generally known reaction partners of water.

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

This information is not available.

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

This information is not available.

Eye irritation

This information is not available.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

Not applicable

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

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

Additional ecological information

No ecological problems are to be expected when the product is handled and used with due care and attention.

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 - 14.6 Not classified as dangerous in the meaning of transport

regulations.

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6 Not classified as dangerous in the meaning of transport

regulations.

Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport

regulations.

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

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

Major Accident Hazard SEVESO III
Legislation Not applicable

Regulation (EC) No 1005/2009 on substances that not regulated

deplete the ozone layer

Regulation (EC) No 850/2004 of the European not regulated Parliament and of the Council of 29 April 2004 on

persistent organic pollutants and amending

Directive 79/117/EEC

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 10 - 13

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.

Training advice

Provide adequate information, instruction and training for operators.

according to Regulation (EC) No. 1907/2006

Catalogue No. 113366

Product name Deuterium oxide deuteration degree min. 99.9% for NMR spectroscopy

MagniSolv™

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.