

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 18.07.2018

Version 15.3

---

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

### 1.1 Product identifier

|                           |  |
|---------------------------|--|
| Catalogue No.             | 102450   |
| Product name              | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |
| REACH Registration Number | 01-2120242098-57-XXXX  |
| CAS-No.                   | 865-49-6   |

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

|                 |   |
|-----------------|---|
| Identified uses | Reagent for analysis<br>In compliance with the conditions described in the annex to this safety data sheet. |
|-----------------|---|

### 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. |
|--------------------------------|---|

---

## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

Acute toxicity, Category 4, Oral, H302  
Acute toxicity, Category 3, Inhalation, H331  
Skin irritation, Category 2, H315  
Eye irritation, Category 2, H319  
Carcinogenicity, Category 2, H351  
Reproductive toxicity, Category 2, H361d  
Specific target organ toxicity - repeated exposure, Category 1, Liver, Kidney, H372  
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*

H302 Harmful if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H331 Toxic if inhaled.  
H351 Suspected of causing cancer.  
H361d Suspected of damaging the unborn child.  
H372 Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure.

*Precautionary statements*

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

breathing.

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

## Reduced labelling (≤125 ml)

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H331 Toxic if inhaled.

H351 Suspected of causing cancer.

H361d Suspected of damaging the unborn child.

H372 Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure.

*Precautionary statements*

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 865-49-6

## 2.3 Other hazards

None known.

---

## SECTION 3. Composition/information on ingredients

### 3.1 Substance

|            |                   |                           |
|------------|-------------------|---------------------------|
| Formula    | CDCl <sub>3</sub> | CCl <sub>3</sub> D (Hill) |
| EC-No.     | 212-742-4         |                           |
| Molar mass | 120,38 g/mol      |                           |

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

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

*Chemical name (Concentration)*

| CAS-No. | Registration number | Classification |
|---------|---------------------|----------------|
|---------|---------------------|----------------|

|                                       |  |  |
|---------------------------------------|--|--|
| Chloroform-D1-Deuteration (<= 100 % ) |  |  |
|---------------------------------------|--|--|

*Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.*

|          |                       |  |
|----------|-----------------------|--|
| 865-49-6 | 01-2120242098-57-XXXX | Acute toxicity, Category 4, H302<br>Acute toxicity, Category 3, H331<br>Skin irritation, Category 2, H315<br>Eye irritation, Category 2, H319<br>Carcinogenicity, Category 2, H351<br>Reproductive toxicity, Category 2, H361d<br>Specific target organ toxicity - repeated exposure, Category 1, H372 |
|----------|-----------------------|--|

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

### 3.2 Mixture

Not applicable

---

## SECTION 4. First aid measures

### 4.1 Description of first aid measures

*General advice*

First aider needs to protect himself.

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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

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

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately. Subsequently administer: activated charcoal (20 - 40 g in 10% slurry).

## 4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Cough, Shortness of breath, Dizziness, agitation, spasms, inebriation, Nausea, Vomiting, Stomach/intestinal disorders, ataxia (impaired locomotor coordination), cardiovascular disorders, Headache, respiratory arrest, narcosis  
Drying-out effect resulting in rough and chapped skin.

## 4.3 Indication of any immediate medical attention and special treatment needed

Laxative: Sodium sulfate (1 tablespoon/1/4 l water).

---

## 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.

Ambient fire may liberate hazardous vapours.

Fire may cause evolution of:

Hydrogen chloride gas, Phosgene

### 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*

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

---

## 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. 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.

### 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. Do not inhale vapours.

### 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*

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

Observe label precautions.

#### *Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### 7.2 Conditions for safe storage, including any incompatibilities

#### *Storage conditions*

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

Protected from light. Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

## 7.3 Specific end use(s)

See exposure scenario in the Annex to this MSDS.

---

## SECTION 8. Exposure controls/personal protection

### 8.1 Control parameters

#### Derived No Effect Level (DNEL)

|                         |                  |            |                        |
|-------------------------|------------------|------------|------------------------|
| Worker DNEL, acute      | Systemic effects | inhalation | 333 mg/m <sup>3</sup>  |
| Worker DNEL, longterm   | Systemic effects | inhalation | 2,5 mg/m <sup>3</sup>  |
| Worker DNEL, longterm   | Systemic effects | dermal     | 0,94 mg/kg Body weight |
| Worker DNEL, longterm   | Local effects    | inhalation | 2,5 mg/m <sup>3</sup>  |
| Consumer DNEL, longterm | Systemic effects | inhalation | 0,18 mg/m <sup>3</sup> |

#### Predicted No Effect Concentration (PNEC)

|                                   |            |
|-----------------------------------|------------|
| PNEC Fresh water                  | 0,146 mg/l |
| PNEC Fresh water sediment         | 0,45 mg/kg |
| PNEC Marine water                 | 0,015 mg/l |
| PNEC Marine sediment              | 0,09 mg/kg |
| PNEC Aquatic intermittent release | 0,133 mg/l |
| PNEC Soil                         | 0,56 mg/kg |
| PNEC Sewage treatment plant       | 0,048 mg/l |

### 8.2 Exposure controls

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## 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:     | Viton (R) |
| Glove thickness:    | 0,70 mm   |
| Break through time: | > 480 min |

splash contact:

|                     |              |
|---------------------|--------------|
| Glove material:     | butyl-rubber |
| Glove thickness:    | 0,7 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 890 Vitoject® (full contact), KCL 898 Butoject® (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](http://www.kcl.de)).



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## *Other protective equipment*

protective clothing

## *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.

---

## **SECTION 9. Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

|                             |  |
|-----------------------------|--|
| Form                        | liquid   |
| Colour                      | colourless   |
| Odour                       | characteristic   |
| Odour Threshold             | No information available.  |
| pH                          | No information available.  |
| Melting point               | -64,1 °C   |
| Boiling point/boiling range | 60 °C<br>at 1.013 hPa  |
| Flash point                 | Method: Tested according to Directive 92/69/EEC.<br>Not applicable |

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

|                  |                           |
|------------------|---------------------------|
| Evaporation rate | No information available. |
|------------------|---------------------------|

|                           |                           |
|---------------------------|---------------------------|
| Flammability (solid, gas) | No information available. |
|---------------------------|---------------------------|

|                       |                |
|-----------------------|----------------|
| Lower explosion limit | Not applicable |
|-----------------------|----------------|

|                       |                |
|-----------------------|----------------|
| Upper explosion limit | Not applicable |
|-----------------------|----------------|

|                 |                     |
|-----------------|---------------------|
| Vapour pressure | 211 hPa<br>at 20 °C |
|-----------------|---------------------|

|                         |                           |
|-------------------------|---------------------------|
| Relative vapour density | No information available. |
|-------------------------|---------------------------|

|         |                                    |
|---------|------------------------------------|
| Density | 1,50 g/cm <sup>3</sup><br>at 20 °C |
|---------|------------------------------------|

|                  |                           |
|------------------|---------------------------|
| Relative density | No information available. |
|------------------|---------------------------|

|                  |  |
|------------------|--|
| Water solubility | 4,6 g/l<br>at 20 °C<br>Method: OECD Test Guideline 105 |
|------------------|--|

|  |   |
|--|---|
| Partition coefficient: n-octanol/water | log Pow: 2 (25 °C)<br>(experimental)<br>(IUCRID) Bioaccumulation is not expected. |
|--|---|

|                           |  |
|---------------------------|--|
| Auto-ignition temperature | > 653 °C<br>Method: Tested according to Directive 92/69/EEC. |
|---------------------------|--|

|                           |  |
|---------------------------|--|
| Decomposition temperature | Distillable in an undecomposed state at normal pressure. |
|---------------------------|--|

|                    |                           |
|--------------------|---------------------------|
| Viscosity, dynamic | No information available. |
|--------------------|---------------------------|

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

|                      |                              |
|----------------------|------------------------------|
| Explosive properties | Not classified as explosive. |
|----------------------|------------------------------|

|                      |      |
|----------------------|------|
| Oxidizing properties | none |
|----------------------|------|

## 9.2 Other data

none

---

## SECTION 10. Stability and reactivity

### 10.1 Reactivity

See section 10.3

### 10.2 Chemical stability

heat-sensitive

Sensitivity to light

### 10.3 Possibility of hazardous reactions

Risk of explosion with:

Ammonia, Amines, nitrogen oxides, bases, Oxygen, alkali amides, organic nitro compounds,  
Alcohols, alkali hydroxides, strong alkalis, Fluorine, peroxi compounds, Alkaline earth metals,  
Alkali metals, Powdered metals

Methanol, with, alcoholates

Methanol, with, strong alkalis

Iron, in powder form

various alloys, sensitive to shock

Methanol, with, Sodium hydroxide

magnesium, in powder form

Oxygen, with, alkali compounds

Aluminium, in powder form

Acetone, with, alkali compounds

Potassium, sensitive to shock

sodium, sensitive to shock

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

Violent reactions possible with:

phosphines, bis(dimethylamino)dimethyl tin, nonmetallic hydrogen compounds, Powdered metals,  
Light metals, Ketones, mineral acids, Strong oxidizing agents, semimetallic hydrogen compounds

## 10.4 Conditions to avoid

no information available

## 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 oral toxicity*

LD50 Rat: 695 mg/kg

(RTECS)

Symptoms: Nausea, Vomiting, Risk of aspiration upon vomiting., Aspiration may cause  
pulmonary oedema and pneumonitis.

*Acute inhalation toxicity*

Acute toxicity estimate: 0,5 mg/l; aerosol

Symptoms: Cough, Shortness of breath, Possible damages:, mucosal irritations, Lung oedema

*Acute dermal toxicity*

LD50 Rabbit: > 3.980 mg/kg

(IUCLID)

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## *Skin irritation*

Rabbit

Result: slight irritation

(IUCLID) (Regulation (EC) No 1272/2008, Annex VI)

Drying-out effect resulting in rough and chapped skin.

Causes skin irritation.

## *Eye irritation*

Rabbit

Result: slight irritation

(IUCLID) (Regulation (EC) No 1272/2008, Annex VI)

Causes serious eye irritation.

## *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.

## *Teratogenicity*

This information is not available.

## *CMR effects*

Carcinogenicity:

Suspected of causing cancer.

Teratogenicity:

Suspected of damaging the unborn child.

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

Causes damage to organs through prolonged or repeated exposure.

Target Organs: Liver, Kidney

## *Aspiration hazard*

This information is not available.

## **11.2 Further information**

Systemic effects:

After absorption:

Dizziness, inebriation, agitation, spasms, narcosis, respiratory arrest

After long-term exposure to the chemical:

drop in blood pressure, Headache, ataxia (impaired locomotor coordination), Stomach/intestinal disorders, cardiovascular disorders

Damage to:

Liver, Kidney, Cardiac

Effect potentiated by: ethanol

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

---

## **SECTION 12. Ecological information**

### **12.1 Toxicity**

#### *Toxicity to fish*

LC50 *Lepomis macrochirus* (Bluegill sunfish): 18 mg/l; 96 h  
(IUCLID)

#### *Toxicity to daphnia and other aquatic invertebrates*

EC50 *Daphnia magna* (Water flea): 79 mg/l; 48 h  
(IUCLID)

EC5 *E.sulcatum*: > 6.560 mg/l; 72 h  
(maximum permissible toxic concentration) (IUCLID)

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## *Toxicity to algae*

IC50 *Scenedesmus quadricauda* (Green algae): 1.100 mg/l; 8 d  
(maximum permissible toxic concentration) (IUCLID)

## *Toxicity to bacteria*

EC50 *Pseudomonas putida*: 125 mg/l; 16 h  
(maximum permissible toxic concentration) (IUCLID)

EC50 activated sludge: 1.010 mg/l; 3 h  
OECD Test Guideline 209

## **12.2 Persistence and degradability**

### *Biodegradability*

0 %; 14 d  
OECD Test Guideline 301C  
Not readily biodegradable.

## **12.3 Bioaccumulative potential**

### *Partition coefficient: n-octanol/water*

log Pow: 2 (25 °C)  
(experimental)

(IUCLID) Bioaccumulation is not expected.

## **12.4 Mobility in soil**

### *Distribution among environmental compartments*

#### Adsorption/Soil

log Koc: 1,72  
(experimental)

Mobile in soils

## **12.5 Results of PBT and vPvB assessment**

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

## **12.6 Other adverse effects**

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## *Henry constant*

14084 Pa·m<sup>3</sup>/mol

Method: (experimental)

(IUCLID) Distribution preferentially in air.

## *Surface tension*

72,3 mN/m

at 20 °C

Method: OECD Test Guideline 115

Discharge into the environment must be avoided.

---

## SECTION 13. Disposal considerations

### *Waste treatment methods*

See [www.retrologistik.com](http://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 1888    |
| 14.2 Proper shipping name         | CHLOROFORM |
| 14.3 Class                        | 6.1        |
| 14.4 Packing group                | III        |
| 14.5 Environmentally hazardous    | --         |
| 14.6 Special precautions for user | yes        |
| Tunnel restriction code           | E          |

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

|                                   |            |
|-----------------------------------|------------|
| 14.1 UN number                    | UN 1888    |
| 14.2 Proper shipping name         | CHLOROFORM |
| 14.3 Class                        | 6.1        |
| 14.4 Packing group                | III        |
| 14.5 Environmentally hazardous    | --         |
| 14.6 Special precautions for user | no         |

## Sea transport (IMDG)

|                                   |            |
|-----------------------------------|------------|
| 14.1 UN number                    | UN 1888    |
| 14.2 Proper shipping name         | CHLOROFORM |
| 14.3 Class                        | 6.1        |
| 14.4 Packing group                | III        |
| 14.5 Environmentally hazardous    | --         |
| 14.6 Special precautions for user | yes        |

|     |         |
|-----|---------|
| EmS | F-A S-A |
|-----|---------|

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           | ACUTE TOXIC<br>H2<br>Quantity 1: 50 t<br>Quantity 2: 200 t |

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

|                           |   |
|---------------------------|---|
| Occupational restrictions | Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable. |
|---------------------------|---|

|   |               |
|---|---------------|
| Regulation (EC) No 1005/2009 on substances that deplete the ozone layer | not regulated |
|---|---------------|

|   |               |
|---|---------------|
| 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 |
|---|---------------|

|  |  |
|--|--|
| 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 | 6.1 D |
|---------------|-------|

## 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.

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

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

|       |   |
|-------|---|
| H302  | Harmful if swallowed.   |
| H315  | Causes skin irritation.   |
| H319  | Causes serious eye irritation.                                  |
| H331  | Toxic if inhaled.   |
| H351  | Suspected of causing cancer.                                    |
| H361d | Suspected of damaging the unborn child.                         |
| H372  | Causes damage to organs through prolonged or repeated exposure. |

## Training advice

Provide adequate information, instruction and training for operators.

## Labelling

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H302 Harmful if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H331 Toxic if inhaled.  
H351 Suspected of causing cancer.  
H361 Suspected of damaging fertility or the unborn child.  
H372 Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure.

*Precautionary statements*

Response

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

## 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](http://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.*

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## EXPOSURE SCENARIO 1 (Industrial use)

---

### 1. Industrial use Reagent for analysis)

#### Sectors of end-use

|              |  |
|--------------|--|
| <i>SU 3</i>  | Industrial uses: Uses of substances as such or in preparations at industrial sites |
| <i>SU9</i>   | Manufacture of fine chemicals  |
| <i>SU 10</i> | Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)       |

#### Chemical product category

|             |                      |
|-------------|----------------------|
| <i>PC19</i> | Intermediate         |
| <i>PC21</i> | Laboratory chemicals |

#### Process categories

|               |   |
|---------------|---|
| <i>PROC1</i>  | Use in closed process, no likelihood of exposure  |
| <i>PROC2</i>  | Use in closed, continuous process with occasional controlled exposure   |
| <i>PROC3</i>  | Use in closed batch process (synthesis or formulation)  |
| <i>PROC8a</i> | Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at non-dedicated facilities |
| <i>PROC8b</i> | Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at dedicated facilities     |
| <i>PROC9</i>  | Transfer of substance or preparation into small containers (dedicated filling line, including weighing)                     |
| <i>PROC15</i> | Use as laboratory reagent   |

#### Environmental Release Categories

|              |   |
|--------------|---|
| <i>ERC1</i>  | Manufacture of substances   |
| <i>ERC6a</i> | Industrial use resulting in manufacture of another substance (use of intermediates) |

---

### 2. Contributing scenarios: Operational conditions and risk management measures

#### 2.1 Contributing scenario controlling environmental exposure for: ERC1

#### Amount used

|                               |            |
|-------------------------------|------------|
| Daily amount per site (Msafe) | 829.589 kg |
|-------------------------------|------------|

---

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## Environment factors not influenced by risk management

|                                 |     |
|---------------------------------|-----|
| Dilution Factor (River)         | 10  |
| Dilution Factor (Coastal Areas) | 100 |

## Other given operational conditions affecting environmental exposure

|                                   |         |
|-----------------------------------|---------|
| Number of emission days per year  | 365     |
| Emission or Release Factor: Air   | 0,07 %  |
| Emission or Release Factor: Water | 0,006 % |

## Conditions and measures related to municipal sewage treatment plant

|   |   |
|---|---|
| Type of Sewage Treatment Plant                  | Municipal sewage treatment plant                      |
| Flow rate of sewage treatment<br>plant effluent | 10.000 m3/d   |
| Percentage removed from waste<br>water          | 85,6 %  |
| Sludge Treatment                                | Sewage sludge should not be applied to natural soils. |

## Conditions and measures related to external treatment of waste for disposal

|                  |   |
|------------------|---|
| Disposal methods | All liquid and solid waste should be incinerated. |
|------------------|---|

---

## 2.2 Contributing scenario controlling environmental exposure for: ERC6a

### Amount used

|                               |          |
|-------------------------------|----------|
| Daily amount per site (Msafe) | 4.800 kg |
|-------------------------------|----------|

## Environment factors not influenced by risk management

|                                 |     |
|---------------------------------|-----|
| Dilution Factor (River)         | 10  |
| Dilution Factor (Coastal Areas) | 100 |

## Other given operational conditions affecting environmental exposure

|                                   |       |
|-----------------------------------|-------|
| Number of emission days per year  | 300   |
| Emission or Release Factor: Air   | 0,5 % |
| Emission or Release Factor: Water | 0,7 % |

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## Conditions and measures related to municipal sewage treatment plant

|   |   |
|---|---|
| Type of Sewage Treatment Plant                  | Municipal sewage treatment plant                      |
| Flow rate of sewage treatment<br>plant effluent | 10.000 m3/d   |
| Percentage removed from waste<br>water          | 85,6 %  |
| Sludge Treatment                                | Sewage sludge should not be applied to natural soils. |

## Conditions and measures related to external treatment of waste for disposal

|                  |   |
|------------------|---|
| Disposal methods | All liquid and solid waste should be incinerated. |
|------------------|---|

---

## 2.3 Contributing scenario controlling worker exposure for: PROC1, PROC2, PROC3, PROC8a, PROC8b, PROC9, PROC15

### Product characteristics

|  |   |
|--|---|
| Concentration of the Substance in<br>Mixture/Article | Covers the percentage of the substance in the product up to<br>100 %. |
| Physical Form (at time of use)                       | High volatile liquid  |

### Frequency and duration of use

|                  |             |
|------------------|-------------|
| Frequency of use | 8 hours/day |
|------------------|-------------|

### Other operational conditions affecting workers exposure

|                  |   |
|------------------|---|
| Outdoor / Indoor | Indoor with local exhaust ventilation (LEV) |
| Outdoor / Indoor | Outdoor                                     |

### Technical conditions and measures

Provide extraction ventilation at points where emissions occur.

### Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

### Conditions and measures related to personal protection, hygiene and health evaluation

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 102450  
Product name Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy  
MagniSolv™

---

Wear suitable gloves (tested to EN374), coverall and eye protection. Wear respiratory protection.

---

## 3. Exposure estimation and reference to its source

### Environment

| CS  | Use descriptor | Msafe         | Compartment      | RCR | Exposure Assessment Method |
|-----|----------------|---------------|------------------|-----|----------------------------|
| 2.1 | ERC1           | 829589 kg/day | All compartments | < 1 | EUSES                      |
| 2.2 | ERC6a          | 4800 kg/day   | All compartments | < 1 | EUSES                      |

### Workers

| CS  | Use descriptor | Exposure duration, route, effect | RCR | Exposure Assessment Method |
|-----|----------------|----------------------------------|-----|----------------------------|
| 2.3 | PROC1          | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC2          | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC3          | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC8a         | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC8b         | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC9          | longterm, combined, systemic     | < 1 | ECETOC TRA                 |
| 2.3 | PROC15         | longterm, combined, systemic     | < 1 | ECETOC TRA                 |

---

## 4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 102450

Product name Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy  
MagniSolv™

---

safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users;  
ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure  
Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH  
Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC  
Guidance Specific Environmental Release Categories (SPERCs).

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

## EXPOSURE SCENARIO 2 (Professional use)

---

### 1. Professional use Reagent for analysis)

#### Sectors of end-use

*SU 22* Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

#### Chemical product category

*PC21* Laboratory chemicals

#### Process categories

*PROC15* Use as laboratory reagent

#### Environmental Release Categories

*ERC6a* Industrial use resulting in manufacture of another substance (use of intermediates)

*ERC8a* Wide dispersive indoor use of processing aids in open systems

---

### 2. Contributing scenarios: Operational conditions and risk management measures

#### 2.1 Contributing scenario controlling environmental exposure for: ERC6a

##### Amount used

|                               |          |
|-------------------------------|----------|
| Daily amount per site (Msafe) | 4.800 kg |
|-------------------------------|----------|

##### Environment factors not influenced by risk management

|                                 |     |
|---------------------------------|-----|
| Dilution Factor (River)         | 10  |
| Dilution Factor (Coastal Areas) | 100 |

##### Other given operational conditions affecting environmental exposure

|                                   |       |
|-----------------------------------|-------|
| Number of emission days per year  | 300   |
| Emission or Release Factor: Air   | 0,5 % |
| Emission or Release Factor: Water | 0,7 % |

##### Conditions and measures related to municipal sewage treatment plant

|                                |                                  |
|--------------------------------|----------------------------------|
| Type of Sewage Treatment Plant | Municipal sewage treatment plant |
| Flow rate of sewage treatment  | 10.000 m3/d                      |

---

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

|               |  |
|---------------|--|
| Catalogue No. | 102450   |
| Product name  | Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy<br>MagniSolv™ |

---

plant effluent

Percentage removed from waste 85,6 %

water

Sludge Treatment Sewage sludge should not be applied to natural soils.

## Conditions and measures related to external treatment of waste for disposal

Disposal methods All liquid and solid waste should be incinerated.

---

## 2.2 Contributing scenario controlling environmental exposure for: ERC8b

### Amount used

Daily amount per site (Msafe) 5 kg

### Environment factors not influenced by risk management

Dilution Factor (River) 10

Dilution Factor (Coastal Areas) 100

### Other given operational conditions affecting environmental exposure

Number of emission days per year 365

### Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant none

### Conditions and measures related to external treatment of waste for disposal

Disposal methods All liquid and solid waste should be incinerated.

---

## 2.3 Contributing scenario controlling worker exposure for: PROC15

### Product characteristics

Concentration of the Substance in Mixture/Article Covers the percentage of the substance in the product up to 100 %.

Physical Form (at time of use) High volatile liquid

### Frequency and duration of use

The Safety Data Sheets for catalogue items are available at [www.merckgroup.com](http://www.merckgroup.com)

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 102450  
Product name Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy  
MagniSolv™

---

Frequency of use 8 hours/day

## Other operational conditions affecting workers exposure

Outdoor / Indoor Indoor with local exhaust ventilation (LEV)

## Technical conditions and measures

Provide extraction ventilation at points where emissions occur.

## Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

## Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves (tested to EN374), coverall and eye protection.

---

## 3. Exposure estimation and reference to its source

### Environment

| CS  | Use descriptor | Msafe       | Compartment      | RCR | Exposure Assessment Method |
|-----|----------------|-------------|------------------|-----|----------------------------|
| 2.1 | ERC6a          | 4800 kg/day | All compartments | < 1 | EUSES                      |
| 2.2 | ERC8b          | < 5 l/day   | All compartments | < 1 | EUSES                      |

### Workers

| CS  | Use descriptor | Exposure duration, route, effect | RCR | Exposure Assessment Method |
|-----|----------------|----------------------------------|-----|----------------------------|
| 2.3 | PROC15         | longterm, combined, systemic     | < 1 | ECETOC TRA                 |

---

## 4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 102450

Product name Chloroform-D1 deuteration degree min. 99.8% for NMR spectroscopy  
MagniSolv™

---

safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users;  
ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure  
Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH  
Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC  
Guidance Specific Environmental Release Categories (SPERCs).