MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 12/12/2012 Version 1.1

SECTION 1. Identification

Product identifier

Product number	102450
Product name	Chloroform-D1 deuteration degree min. 99.8% 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

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

SECTION 2. Hazards identification

GHS Classification

Carcinogenicity, Category 2, H351
Acute toxicity, Category 4, Oral, H302
Specific target organ systemic toxicity - repeated exposure, Category 2, H373
Skin irritation, Category 2, H315

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

GHS-Labeling

Hazard pictograms

Signal Word
Warning

Hazard Statements
H351 Suspected of causing cancer.
H302 Harmful if swallowed.
H373 May cause damage to organs through prolonged or repeated exposure.
H315 Causes skin irritation.

Precautionary Statements
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P314 Get medical advice/ attention if you feel unwell.

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	$CDCl_3$	CCl_3D (Hill)
CAS-No.	865-49-6	
Molar mass	120.38 g/mol	

Hazardous ingredients
Chemical Name (Concentration)
CAS-No.

Chloroform-D1-Deuteration (<= 100 %)
865-49-6

SECTION 4. First aid measures

Description of first-aid measures
Inhalation
After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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
If swallowed Caution Aspiration hazard Keep respiratory tract clear. Call a physician immediately. Subsequently administer: activated charcoal (20 - 40 g in 10% slurry). In case of spontaneous vomiting: Risk of aspiration. Pulmonary failure possible. Call in physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

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

Indication of any immediate medical attention and special treatment needed
Laxative: Sodium sulfate (1 tablespoon/1/4 l water).

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture
Not combustible.
Ambient fire may liberate hazardous vapors.
Fire may cause evolution of:
Hydrogen chloride gas, Phosgene

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

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, 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.

Environmental precautions
Do not empty into drains.

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 vapors.

SECTION 7. Handling and storage

Precautions for safe handling

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

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Protected from light. Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Store at +2°C to +8°C (+36°F to +46°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
Chloroform-D1-Deuteration 865-49-6			
ACGIH	Time Weighted Average (TWA):	10 ppm	
NIOSH/GUIDE	Short Term Exposure Limit (STEL):	2 ppm 9.78 mg/m³	
OSHA_TRANS	Ceiling Limit Value:	50 ppm 240 mg/m³	
Z1A	Time Weighted Average (TWA):	2 ppm 9.78 mg/m³	

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.

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:

protective clothing

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	No information available.
pH	No information available.
Melting point	-83.4 °F (-64.1 °C)
Boiling point/boiling range	140 °F (60 °C)
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	not applicable
Upper explosion limit	not applicable
Vapor pressure	211 hPa at 68 °F (20 °C)
Relative vapor density	No information available.
Relative density	1.50 g/cm³ at 68 °F (20 °C)
Water solubility	8.2 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 2 (25 °C) (experimental) (IUCLID) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.

Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.

SECTION 10. Stability and reactivity

Reactivity
See below

Chemical stability
heat-sensitive
Sensitivity to light

Possibility of hazardous reactions
Risk of explosion with:

metal alloys, magnesium, Aluminum, Iron, Ammonia, Amines, nitrogen oxides, bases, Oxygen, alkali amides, organic nitro compounds, Alcohols, alkali hydroxides, Methanol, Sodium hydroxide, strong alkalis, alcoholates, Fluorine, peroxi compounds, Alkaline earth metals, Alkali metals

Violent reactions possible with:

phosphines, bis(dimethylamino)dimethyl tin, nonmetallic hydrogen compounds, Powdered metals

Conditions to avoid
Strong heating.

Incompatible materials
rubber, various plastics

Hazardous decomposition products
in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Inhalation, Eye contact, Skin contact

Target Organs
Liver
Kidneys
Heart
Eyes
Skin
Central nervous system

Acute oral toxicity
LD50 rat: 695 mg/kg (RTECS)

LDLO human: 2,514 mg/kg (RTECS)
Symptoms: Nausea, Vomiting, Aspiration may cause pulmonary edema and pneumonitis.
absorption

Acute inhalation toxicity
LCLO human: 124.1 mg/l; 5 min (RTECS)
Symptoms: Cough, Shortness of breath
absorption
LC50 rat: 47.7 mg/l; 4 h (IUCLID)

Acute dermal toxicity
absorption

Skin irritation
rabbit
Result: slight irritation
(IUCLID) Drying-out effect resulting in rough and chapped skin.
Causes skin irritation.

Eye irritation
rabbit
Result: slight irritation
(IUCLID)

CMR effects
Carcinogenicity:
Suspected of causing cancer.

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
May cause damage to organs through prolonged or 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

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
Further data:
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

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)

Toxicity to algae
IC5 Scenedesmus quadricauda (Green algae): 1,100 mg/l; 8 d (maximum permissible toxic concentration) (IUCLID)

Toxicity to bacteria
EC5 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

Persistence and degradability

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

Bioaccumulative potential

Partition coefficient: n-octanol/water
log Pow: 2 (25 °C)
(experimental)
(IUCLID) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Henry constant
14084 Pa*m³/mol
(experimental) (IUCLID) Distribution preferentially in air.

Additional ecological information
Biological effects:
Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.
Further information on ecology
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 1888
Proper shipping name	CHLOROFORM
Class	6.1
Packing group	III
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 1888
Proper shipping name	CHLOROFORM
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 1888
Proper shipping name	CHLOROFORM
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-A

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Skin irritant
Carcinogen
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

Acute Health Hazard
Chronic Health Hazard

US State Regulations

Massachusetts Right To Know

Ingredients
Chloroform-D1-Deuteration

Pennsylvania Right To Know

Ingredients
Chloroform-D1-Deuteration

New Jersey Right To Know

Ingredients
Chloroform-D1-Deuteration

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:	All components of this product are on the Canadian DSL.

SECTION 16. Other information

Details in analogy to the undeuterated compound.

Training advice

Provide adequate information, instruction and training for operators.

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

H302	Harmful if swallowed.
H315	Causes skin irritation.
H351	Suspected of causing cancer.
H373	May cause damage to organs through prolonged or repeated exposure.

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.

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