

according to Regulation (EC) No. 1907/2006

Revision Date 21.06.2018

Version 13.0

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

#### 1.1 Product identifier

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

REACH Registration Number 01-2119457603-38-XXXX

CAS-No. 142-82-5

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

Identified uses Reagent for analysis, Solvent

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)

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

Flammable liquid, Category 2, H225

Skin irritation, Category 2, H315

Specific target organ toxicity - single exposure, Category 3, Central nervous system, H336

Aspiration hazard, Category 1, H304

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

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.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H336 May cause drowsiness or dizziness.

H410 Very toxic to aquatic life with long lasting effects.

## Precautionary statements

#### Prevention

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

P240 Ground/bond container and receiving equipment.

P273 Avoid release to the environment.

#### Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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

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Product name n-Heptane for liquid chromatography LiChrosolv®

#### Storage

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

#### Reduced labelling (≤125 ml)

Hazard pictograms









Signal word

Danger

Hazard statements

H304 May be fatal if swallowed and enters airways.

Precautionary statements

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

*Index-No.* 601-008-00-2

## 2.3 Other hazards

None known.

#### **SECTION 3. Composition/information on ingredients**

#### 3.1 Substance

Formula  $CH_3(CH_2)_5CH_3$   $C_7H_{16}$  (Hill)

Index-No. 601-008-00-2

EC-No. 205-563-8

Molar mass 100,2 g/mol

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

Chemical name (Concentration)

CAS-No. Registration number Classification

n-heptane (<= 100 %)

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

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## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

XXXX Flammable liquid, Category 2, H225

Skin irritation, Category 2, H315

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

Aspiration hazard, Category 1, H304

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

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

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. Remove contact lenses.

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

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

irritant effects, Drowsiness, Unconsciousness, narcosis, Headache, somnolence, Vertigo, death

## 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.

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#### 5.2 Special hazards arising from the substance or mixture

Combustible.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

## 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.

#### **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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

#### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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Product name n-Heptane for liquid chromatography LiChrosolv®

## **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

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

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)

See exposure scenario in the Annex to this MSDS.

## **SECTION 8. Exposure controls/personal protection**

## 8.1 Control parameters

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

#### **Derived No Effect Level (DNEL)**

Worker DNEL, longterm Systemic effects inhalation 2085 mg/m³

Worker DNEL, longterm Systemic effects dermal 300 mg/kg Body weight

Consumer DNEL, longterm Systemic effects inhalation 447 mg/m³

Consumer DNEL, longterm Systemic effects dermal 149 mg/kg Body weight

Consumer DNEL, longterm Systemic effects oral 149 mg/kg Body weight

#### **Predicted No Effect Concentration (PNEC)**

PNEC no data available

#### 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

Safety glasses

Hand protection

full contact:

Glove material: Nitrile rubber
Glove thickness: 0,40 mm
Break through time: 480 min

splash contact:

Glove material: Nitrile rubber

## according to Regulation (EC) No. 1907/2006

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Product name n-Heptane for liquid chromatography LiChrosolv®

Glove thickness: 0,2 mm

Break through time: 60 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 730 Camatril® -Velours (full contact), KCL 743 Dermatril® P (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.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds. The entrepeneur 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

# according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

Odour Threshold No information available.

pH No information available.

Melting point -90,5 °C

Boiling point/boiling range 97 - 98 °C

at 1.013 hPa

Flash point -4 °C

Method: c.c.

Evaporation rate No information available.

Flammability (solid, gas) No information available.

Lower explosion limit 1 %(V)

Upper explosion limit 7 %(V)

Vapour pressure 48 hPa

at 20 °C

Relative vapour density 3,46

Density 0,68 g/cm3

at 20 °C

Relative density No information available.

Water solubility 0,05 g/l

at 20 °C

## according to Regulation (EC) No. 1907/2006

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Product name n-Heptane for liquid chromatography LiChrosolv®

Partition coefficient: n- log Pow: 4,66 octanol/water (experimental)

(Lit.) Potential bioaccumulation

Auto-ignition temperature No information available.

Decomposition temperature No information available.

Viscosity, dynamic 0,42 mPa.s

at 20 °C

Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

Ignition temperature 215 °C

Minimum ignition energy 0,24 mJ

## **SECTION 10. Stability and reactivity**

#### 10.1 Reactivity

Vapours may form explosive mixture with air.

Vapours may form explosive mixture with air.

#### 10.2 Chemical stability

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

#### 10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Strong oxidizing agents

phosphorus, in the presence of:

Chlorine

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Product name n-Heptane for liquid chromatography LiChrosolv®

#### 10.4 Conditions to avoid

Warming.

Warming.

## 10.5 Incompatible materials

rubber, various plastics

#### 10.6 Hazardous decomposition products

no information available

no information available

## **SECTION 11. Toxicological information**

## 11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 5.000 mg/kg OECD Test Guideline 401

Symptoms: Irritation of mucous membranes

Acute inhalation toxicity

LC50 Rat: > 29,3 g/m3; 4 h; vapour

**OECD Test Guideline 403** 

Symptoms: Irritation symptoms in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: > 2.000 mg/kg OECD Test Guideline 402

Skin irritation

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Causes skin irritation.

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Product name n-Heptane for liquid chromatography LiChrosolv®

Eye irritation

Rabbit

Result: No eye irritation

(IUCLID)

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

**Teratogenicity** 

This information is not available.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Target Organs: Central nervous system

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

#### 11.2 Further information

After uptake of large quantities:

Headache, Vertigo, Unconsciousness, narcosis, death

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Product name n-Heptane for liquid chromatography LiChrosolv®

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

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 Carassius auratus (goldfish): 4 mg/l; 24 h
ASTM D1345
(Lit.)
```

## 12.2 Persistence and degradability

```
Biodegradability
70 %; 10 d; aerobic
(ECHA)
Readily biodegradable
Biochemical Oxygen Demand (BOD)
1.920 mg/g (5 d)

(IUCLID)
Theoretical oxygen demand (ThOD)
3.500 mg/g

(Lit.)
Ratio BOD/ThBOD
BOD5 55 %
(Lit.)
```

## 12.3 Bioaccumulative potential

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

Partition coefficient: n-octanol/water

log Pow: 4,66 (experimental)

(Lit.) Potential bioaccumulation

## 12.4 Mobility in soil

No information available.

## 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

Henry constant

208678 Pa\*m3/mol

Method: (calculated)

(Lit.) Distribution preferentially in air.

Discharge into the environment must be avoided.

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

## **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 1206

14.2 Proper shipping name HEPTANES

**14.3 Class** 3

14.4 Packing group

14.5 Environmentally hazardous yes

14.6 Special precautions for yes

user

Tunnel restriction code D/E

#### Inland waterway transport (ADN)

Not relevant

## Air transport (IATA)

**14.1 UN number** UN 1206

14.2 Proper shipping name HEPTANES

**14.3 Class** 3

14.4 Packing group

14.5 Environmentally hazardous yes

**14.6 Special precautions for** no

user

Sea transport (IMDG)

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

**14.1 UN number** UN 1206

14.2 Proper shipping name HEPTANES

**14.3 Class** 3

14.4 Packing group

14.5 Environmentally hazardous yes

**14.6 Special precautions for** yes

user

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 ENVIRONMENTAL HAZARDS

E1

Quantity 1: 100 t Quantity 2: 200 t

Occupational restrictions

Take note of Dir 94/33/EC on the protection of young people at

work.

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

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

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**

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

H225 Highly flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H336 May cause drowsiness or dizziness.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

## Training advice

Provide adequate information, instruction and training for operators.

## Labelling

Hazard pictograms









Signal word

Danger

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

#### Hazard statements

H225 Highly flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H336 May cause drowsiness or dizziness.

H410 Very toxic to aquatic life with long lasting effects.

#### Precautionary statements

Prevention

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

P240 Ground/bond container and receiving equipment.

P273 Avoid release to the environment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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

P313 Get medical advice/ attention.

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.

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

#### **EXPOSURE SCENARIO 1 (Industrial use)**

## 1. Industrial use Reagent for analysis, Solvent)

#### Sectors of end-use

SU 3 Industrial uses: Uses of substances as such or in preparations at industrial sites

SU9 Manufacture of fine chemicals

SU 10 Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)

#### Chemical product category

PC19 Intermediate

PC21 Laboratory chemicals

#### **Process categories**

PROC1	Use in closed process, no likelihood of exposure
PROC2	Use in closed, continuous process with occasional controlled exposure

PROC3 Use in closed batch process (synthesis or formulation)

PROC4 Use in batch and other process (synthesis) where opportunity for exposure arisesPROC5 Mixing or blending in batch processes for formulation of preparations and articles

(multistage and/ or significant contact)

PROC8a Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large

containers at non-dedicated facilities

PROC8b Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large

containers at dedicated facilities

PROC9 Transfer of substance or preparation into small containers (dedicated filling line, including

weighing)

PROC10 Roller application or brushing

PROC15 Use as laboratory reagent

#### **Environmental Release Categories**

ERC1	Manufacture of substances
ERC2	Formulation of preparations

ERC4 Industrial use of processing aids in processes and products, not becoming part of articles

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

ERC6b Industrial use of reactive processing aids

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Product name n-Heptane for liquid chromatography LiChrosolv®

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

#### 2.1 Contributing scenario controlling environmental exposure for: ERC1, ERC4, SpERC ESVOC 1

#### Amount used

Daily amount per site (Msafe) 330 t

#### 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 100
Emission or Release Factor: Air 5 %
Emission or Release Factor: Water 0,03 %
Emission or Release Factor: Soil 0,01 %

#### Technical conditions and measures / Organizational measures

Air Use of air emission abatement equipments.

Effectiveness (of a measure): 90 %

Water Ensure all waste water is collected and treated via a WWTP.

## Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 10.000 m3/d

plant effluent

Percentage removed from waste 96,2 %

water

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

sludge should be incinerated.

#### 2.2 Contributing scenario controlling environmental exposure for: ERC2, SpERC ESVOC 4

#### Amount used

Daily amount per site (Msafe) 99 t

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

#### 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 100

Emission or Release Factor: Air 2,5 %

Emission or Release Factor: Water 0,02 %

Emission or Release Factor: Soil 0,01 %

#### Technical conditions and measures / Organizational measures

Water Ensure all waste water is collected and treated via a WWTP.

## Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 2.000 m3/d

plant effluent

Percentage removed from waste 96,2 %

water

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

sludge should be incinerated.

#### 2.3 Contributing scenario controlling environmental exposure for: ERC6a, ERC6b, SpERC ESVOC 3

## Amount used

Daily amount per site (Msafe) 540 t

## 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 20
Emission or Release Factor: Air 0,1 %
Emission or Release Factor: Water 0,001 %

# according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

Emission or Release Factor: Soil 0,001 %

#### Technical conditions and measures / Organizational measures

Air Use of air emission abatement equipments.

Effectiveness (of a measure): 90 %

Water Ensure all waste water is collected and treated via a WWTP.

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

Flow rate of sewage treatment 2.000 m3/d

plant effluent

Percentage removed from waste

96,2 %

water

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

sludge should be incinerated.

# 2.4 Contributing scenario controlling worker exposure for: PROC1, PROC2, PROC3, PROC4, PROC5, PROC8a, PROC8b, PROC9, PROC10, PROC15

#### **Product characteristics**

Concentration of the Substance in Covers the percentage of the substance in the product up to

Mixture/Article 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 without local exhaust ventilation (LEV)

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

Covers daily exposures up to 8 hours.

#### Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Wear suitable gloves (tested to EN374) and eye protection.

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Ensure adequate ventilation.

## 3. Exposure estimation and reference to its source

## **Environment**

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC1, ERC4	330 t/day	Fresh water sediment	< 1	Petrorisk
2.2	ERC2	99 t/day	Fresh water sediment	< 1	Petrorisk
2.3	ERC6a, ERC6b	540 t/day	Fresh water	< 1	Petrorisk

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Product name n-Heptane for liquid chromatography LiChrosolv®

#### **Workers**

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.4	PROC1	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC2	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC3	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4 F	PROC4	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC5	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC8a	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC8b	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC9	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC10	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	
2.4	PROC15	longterm, inhalative, systemic	< 1	ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

according to Regulation (EC) No. 1907/2006

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Product name n-Heptane for liquid chromatography LiChrosolv®

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

according to Regulation (EC) No. 1907/2006

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Product name n-Heptane for liquid chromatography LiChrosolv®

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

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool ScIDeEx® at www.merckmillipore.com/scideex.

## according to Regulation (EC) No. 1907/2006

Catalogue No. 104390

Product name n-Heptane for liquid chromatography LiChrosolv®

#### **EXPOSURE SCENARIO 2 (Professional use)**

## 1. Professional use Reagent for analysis, Solvent)

#### 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**

ERC2 Formulation of preparations

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

ERC6b Industrial use of reactive processing aids

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

## 2.1 Contributing scenario controlling environmental exposure for: ERC2, SpERC ESVOC 4

#### Amount used

Daily amount per site (Msafe) 99 t

#### 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 100
Emission or Release Factor: Air 2,5 %
Emission or Release Factor: Water 0,02 %
Emission or Release Factor: Soil 0,01 %

## Technical conditions and measures / Organizational measures

Water Ensure all waste water is collected and treated via a WWTP.

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## Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 2.000 m3/d

plant effluent

Percentage removed from waste 96,2 %

water

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

sludge should be incinerated.

## 2.2 Contributing scenario controlling environmental exposure for: ERC6a, ERC6b, SpERC ESVOC 3

#### Amount used

Daily amount per site (Msafe) 540 t

#### 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 20
Emission or Release Factor: Air 0,1 %
Emission or Release Factor: Water 0,001 %
Emission or Release Factor: Soil 0,001 %

#### Technical conditions and measures / Organizational measures

Air Use of air emission abatement equipments.

Effectiveness (of a measure): 90 %

Water Ensure all waste water is collected and treated via a WWTP.

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

Flow rate of sewage treatment 2.000 m3/d

plant effluent

Percentage removed from waste 96,2 %

water

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

sludge should be incinerated.

#### 2.3 Contributing scenario controlling worker exposure for: PROC15

#### **Product characteristics**

Concentration of the Substance in Covers the percentage of the substance in the product up to

Mixture/Article 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 without local exhaust ventilation (LEV)

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

Covers daily exposures up to 8 hours.

#### Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Wear suitable gloves (tested to EN374) and eye protection.

Ensure adequate ventilation.

#### 3. Exposure estimation and reference to its source

#### **Environment**

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC2	99 t/day	Fresh water sediment	< 1	Petrorisk
2.2	ERC6a, ERC6b	540 t/day	Fresh water	< 1	Petrorisk

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#### Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.3	PROC15	longterm, inhalative, systemic		ECETOC TRA 3
		longterm, dermal, systemic	< 1	ECETOC TRA 3
		longterm, combined, systemic	< 1	

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

# 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 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).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool ScIDeEx® at www.merckmillipore.com/scideex.