

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Date of issue: 01.11.2016

Version 1.0

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No.	103701
Product name	n-Hexane hypergrade for LC-MS LiChrosolv®
REACH Registration Number	01-2119480412-44-XXXX
CAS-No.	110-54-3

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

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

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

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification**2.1 Classification of the substance or mixture**

Classification (REGULATION (EC) No 1272/2008)

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Product name n-Hexane hypergrade for LC-MS LiChrosolv®

Flammable liquid, Category 2, H225
Skin irritation, Category 2, H315
Reproductive toxicity, Category 2, H361fd
Specific target organ toxicity - single exposure, Category 3, Central nervous system, H336
Specific target organ toxicity - repeated exposure, Category 2, Inhalation, Nervous system, H373
Aspiration hazard, Category 1, H304
Chronic aquatic toxicity, Category 2, H411

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.
H361fd Suspected of damaging fertility. Suspected of damaging the unborn child.
H373 May cause damage to organs (Nervous system) through prolonged or repeated exposure if inhaled.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. 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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P314 Get medical advice/ attention if you feel unwell.

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.

H361fd Suspected of damaging fertility. Suspected of damaging the unborn child.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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

Index-No. 601-037-00-0

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ (CH ₂) ₄ CH ₃	C ₆ H ₁₄ (Hill)
Index-No.	601-037-00-0	
EC-No.	203-777-6	
Molar mass	86,18 g/mol	

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

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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n-Hexane (<= 100 %)

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

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Specific target organ toxicity - single exposure, Category 3, H336
Specific target organ toxicity - repeated exposure, Category 2,
H373
Aspiration hazard, Category 1, H304
Chronic aquatic toxicity, Category 2, H411

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. Consult a physician.

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

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

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, somnolence, Drowsiness

narcosis, Nausea, Tiredness, CNS disorders, paralysis symptoms

Risk of corneal clouding.

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.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

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SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

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

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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.

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.

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)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

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Derived No Effect Level (DNEL)

Worker DNEL, longterm	Systemic effects	inhalation	75 mg/m ³
Worker DNEL, longterm	Systemic effects	dermal	16 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	dermal	5,3 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	oral	4 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
Glove thickness:	0,11 mm
Break through time:	> 10 min

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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 741 Dermatril® L (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 entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	benzine-like
Odour Threshold	No information available.
pH	Not applicable
Melting point	-94,3 °C

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Boiling point/boiling range	69 °C at 1.013 hPa
Flash point	-22 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,0 %(V)
Upper explosion limit	8,1 %(V)
Vapour pressure	160 hPa at 20 °C
Relative vapour density	2,79
Density	0,66 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,0095 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 4,11 (calculated) (Lit.) Potential bioaccumulation
Auto-ignition temperature	No information available.
Decomposition temperature	Distillable in an undecomposed state at normal pressure.
Viscosity, dynamic	0,326 mPa.s at 20 °C

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Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

Ignition temperature 240 °C
Method: DIN 51794

Viscosity, kinematic 0,50 mm²/s
at 20 °C

SECTION 10. Stability and reactivity

10.1 Reactivity

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 explosion with:

Strong oxidizing agents, nitrogen oxides

Violent reactions possible with:

halogens

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

SODIUM PEROXIDE

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 16.000 mg/kg
OECD Test Guideline 401

Symptoms: Nausea

Acute inhalation toxicity

LC50 Rat: 172 mg/l; 4 h ; vapour
(RTECS)

Symptoms: Irritation symptoms in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: > 2.000 mg/kg
(ECHA)

absorption

Skin irritation

Causes skin irritation.

Eye irritation

Risk of corneal clouding.

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vivo

Micronucleus test
Result: negative

(National Toxicology Program)

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Genotoxicity in vitro

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: Positive results were obtained in some in vitro tests.

Method: OECD Test Guideline 476

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.

CMR effects

Teratogenicity:

Suspected of damaging the unborn child.

Reproductive toxicity:

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Target Organs: Central nervous system

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Exposure routes: Inhalation

Target Organs: Nervous system

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Further information

After absorption:

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Tiredness, narcosis

After long-term exposure to the chemical:

CNS disorders, paralysis symptoms

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.

This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 2,5 mg/l; 96 h
(ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 2,1 mg/l; 48 h
(Lit.)

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 4,11
(calculated)

(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

183000 Pa*m³/mol

(HSDB) Distribution preferentially in air.

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Discharge into the environment must be avoided.

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 1208
14.2 Proper shipping name	HEXANES
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1208
14.2 Proper shipping name	HEXANES
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 1208
14.2 Proper shipping name	HEXANES
14.3 Class	3
14.4 Packing group	II

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14.5 Environmentally hazardous yes

14.6 Special precautions for user yes

EmS F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard SEVESO III
Legislation ENVIRONMENTAL HAZARDS

E2
Quantity 1: 200 t
Quantity 2: 500 t

SEVESO III
FLAMMABLE LIQUIDS
P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. 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

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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of ≥ 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.
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure if inhaled.
H411	Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

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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.
H361 Suspected of damaging fertility or the unborn child.
H373 May cause damage to organs (Nervous system, Central nervous system) through prolonged or repeated exposure if inhaled.
H411 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.
P314 Get medical advice/ attention if you feel unwell.

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.