

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 29.01.2018

Version 12.0

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

Catalogue No.	104365
Product name	n-Heptane EMPLURA®
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	Chemical production, Solvent In compliance with the conditions described in the annex to this safety data sheet.
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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)**

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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) ₅ CH ₃	C ₇ H ₁₆ (Hill)
Index-No.	601-008-00-2	
EC-No.	205-563-8	
Molar mass	100,2 g/mol	

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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.

142-82-5 01-2119457603-38-

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. Consult doctor if feeling unwell.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary. Remove contact lenses.

If swallowed Caution Aspiration hazard Keep respiratory tract clear. Call a physician immediately. In case of spontaneous vomiting: Risk of aspiration. Pulmonary failure possible. Call in physician.

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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.

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Pay attention to flashback.

Forms explosive mixtures with air at ambient temperatures.

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

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. Remove container from danger zone and cool with water.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapours, aerosols. Keep away from heat and sources of ignition. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

6.2 Environmental precautions

Do not empty into 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 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)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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, longterm	Systemic effects	inhalation	2085 mg/m ³
Worker DNEL, longterm	Systemic effects	dermal	300 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	inhalation	447 mg/m ³
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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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: 0,2 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 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 empty into drains.

Risk of explosion.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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	-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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

Density	0,68 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,05 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 4,66 (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.

10.2 Chemical stability

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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.

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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

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)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

Theoretical oxygen demand (ThOD)

3.500 mg/g

(Lit.)

Ratio BOD/ThBOD

BOD5 55 %

(Lit.)

12.3 Bioaccumulative potential

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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	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 1206
14.2 Proper shipping name	HEPTANES
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

14.1 UN number UN 1206

14.2 Proper shipping name HEPTANES

14.3 Class 3

14.4 Packing group II

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 FLAMMABLE LIQUIDS

P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

SEVESO III
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 deplete the ozone layer not regulated

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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 ≥ 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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

Labelling

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.
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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	104365
Product name	n-Heptane EMPLURA®

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. 104365
Product name n-Heptane EMPLURA®

EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use Chemical production, Solvent)

Sectors of end-use

- SU 3* Industrial uses: Uses of substances as such or in preparations at industrial sites
SU 9 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 arises
PROC5 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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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 %

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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 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

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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	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).

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	104365
Product name	n-Heptane EMPLURA®

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

EXPOSURE SCENARIO 2 (Professional use)

1. Professional use Chemical production, Solvent)

Sectors of end-use

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

Chemical product category

PC 21 Laboratory chemicals

Process categories

PROC 15 Use as laboratory reagent

Environmental Release Categories

ERC 2 Formulation of preparations

ERC 6a Industrial use resulting in manufacture of another substance (use of intermediates)

ERC 6b 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.

SAFETY DATA SHEET

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Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment plant effluent 2.000 m³/d
Percentage removed from waste water 96,2 %
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 plant effluent 2.000 m³/d
Percentage removed from waste water 96,2 %

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

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 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

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104365
Product name n-Heptane EMPLURA®

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.3	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).

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).

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