

Safety Data Sheet

According to EC Directive 91/155/EEC

Date of issue: 19.02.2004
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1. Identification of the substance/preparation and of the company/undertaking

Identification of the product

Catalogue No.: 104365
Product name: n-Heptane extra pure

Use of the substance/preparation

Chemical production
Solvent

Company/undertaking identification

Company: Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Emergency telephone No.: Please contact the regional Merck representation in your country.

2. Composition/information on ingredients

Synonyms

n-Dipropylmethane, n-Heptylhydride

CAS-No.:	142-82-5	EC-Index-No.:	601-008-00-2
M:	100.21 g/mol	EC-No.:	205-563-8
Formula Hill:	C ₇ H ₁₆		
Chemical formula:	CH ₃ (CH ₂) ₅ CH ₃		

3. Hazards identification

Highly flammable. Irritating to skin. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. Harmful: may cause lung damage if swallowed. Vapours may cause drowsiness and dizziness.

4. 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.
After swallowing: Avoid vomiting. Risk of aspiration! Immediately call in physician.

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5. Fire-fighting measures

Suitable extinguishing media:
powder, foam.

Special risks:
Combustible. Vapours heavier than air. Forms explosive mixtures with air at ambient temperatures. Development of hazardous combustion gases or vapours possible in the event of fire.

Special protective equipment for fire fighting:
Do not stay in dangerous zone without self-contained breathing apparatus. In order to avoid contact with skin, keep a safety distance and wear suitable protective clothing.

Other information:
Take measures to prevent electrostatic charging. Prevent fire-fighting water from entering surface water or groundwater.

6. Accidental release measures

Person-related precautionary measures:
Avoid substance contact. Do not inhale vapours/aerosols. Ensure supply of fresh air in enclosed rooms.

Environmental-protection measures:
Do not allow to enter sewerage system; risk of explosion!

Procedures for cleaning / absorption:
Take up with liquid-absorbent material (e.g. Chemisorb®). Forward for disposal. Clean up affected area.

7. Handling and storage

Handling:

Notes for prevention of fire and explosion:
Keep away from sources of ignition. Take measures to prevent electrostatic charging.

Notes for safe handling:
Work under hood. Do not inhale substance. Avoid generation of vapours/aerosols.

Storage:

Tightly closed in a well-ventilated place, away from sources of ignition and heat. Storage temperature: no restrictions.

8. Exposure controls/personal protection

Specific control parameter

EC

Name	n-Heptane
Value	500 ml/m ³
	2085 mg/m ³

Personal protective equipment:

Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled. The resistance of the protective clothing to chemicals should be ascertained with the respective supplier.

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Respiratory protection: required when vapours/aerosols are generated. Filter A (acc. to DIN 3181) for vapours of organic compounds.

Eye protection: required

Hand protection:

In full contact:

Glove material: nitrile rubber

Layer thickness: 0.40 mm

Breakthrough time: > 480 Min.

In splash contact:

Glove material: polychloroprene

Layer thickness: 0.65 mm

Breakthrough time: > 60 Min.

The protective gloves to be used must comply with the specifications of EC directive 89/686/EEC and the resultant standard EN374, for example KCL 730 Camatril® -Velours (full contact), 720 Camapren® (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 and supplied by us as well as to the purpose specified by us. 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).

Industrial hygiene:

Change contaminated clothing. Apply skin-protective barrier cream. Wash hands after working with substance. Work under hood. Do not inhale substance.

9. Physical and chemical properties

Form:	liquid		
Colour:	colourless		
Odour:	characteristic		
pH value		not available	
Viscosity dynamic	(20 °C)	0.42	mPa*s
Melting point		-90.6	°C
Boiling point	(1013 hPa)	98.4	°C
Ignition temperature		215	°C
Flash point		-4	°C c.c.
Explosion limits	lower	1	Vol%
	upper	7	Vol%
Vapour pressure	(20 °C)	48	hPa
Relative vapour density		3.46	
Density	(20 °C)	0.68	g/cm ³
Solubility in water	(20 °C)	almost insoluble	
log Pow:		4.66	
Bioconcentration factor		340-2000	(calculated)

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10. Stability and reactivity

Conditions to be avoided

Heating.

Substances to be avoided

strong oxidizing agents.

Hazardous decomposition products

no information available

Further information

highly inflammable;
unsuitable working materials: various plastics, rubber.
Explosible with air in a vaporous/gaseous state.

11. Toxicological information

Acute toxicity

LC₅₀ (inhalation, rat): 103 g/m³ /4 h.
LD₅₀ (oral, rat): >15000 mg/kg.

Specific symptoms in animal studies:
Eye irritation test (rabbit): Slight irritations.

Subacute to chronic toxicity

No indication of mutagenic activity.
Bacterial mutagenicity: Ames test: negative.

Further toxicological information

After inhalation of vapours/aerosols: Irritation symptoms in the respiratory tract. drowsiness, drowsiness.

After skin contact: Irritations. Degreasing effect on the skin, possibly followed by secondary inflammation.

After eye contact: Slight irritations.

After swallowing: irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract. headache, drowsiness, drowsiness, dizziness, unconsciousness, narcosis (death). respiratory arrest. After accidental swallowing the substance may pose a risk of aspiration. Passage into the lung (vomiting!) can result in a condition resembling pneumonia (chemical pneumonitis).

Other notes:

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.

Further data

The product should be handled with the care usual when dealing with chemicals.

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12. Ecological information

Behavior in environmental compartments:

Concentration in organisms possible.

Distribution: log p(o/w): 4.66.

An appreciable bioaccumulation potential is to be expected (log P(o/w) >3).

Henry constant: 278730 Pa*m³/mol (volatile).

BCF: 340-2000 (calculated).

Ecotoxic effects:

Biological effects:

Highly toxic for aquatic organisms. May cause long-term adverse effects in the aquatic environment.

Fish toxicity: C.auratus LC₅₀: 4 mg/l /24 h.

Daphnia toxicity: Daphnia magna EC₅₀: 1.5 mg/l /48 h.

The literature data available to us do not conform with the labelling prescribed by the EC. The EC has dossiers which have not been published.

Further ecologic data:

BOD 55 % from TOD /5 d. TOD: 3.5 g/g.

Do not allow to enter waters, waste water, or soil!

13. Disposal considerations

Product:

Chemicals must be disposed of in compliance with the respective national regulations. Under www.retrologistik.de you will find country- and substance-specific information as well as contact partners.

Packaging:

Merck product packaging must be disposed of in compliance with the country-specific regulations or must be passed to a packaging return system. Under www.retrologistik.de you will find special information on the respective national conditions as well as contact partners.

14. Transport information

Road & Rail ADR, RID

UN 1206 HEPTANE, 3, II

Inland waterway ADN, ADNR not tested

Sea IMDG-Code

UN 1206 HEPTANES, 3, II

Ems F-E S-D

Air CAO, PAX

HEPTANES, 3, UN 1206, II

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

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15. Regulatory information

Labelling according to EC Directives

Symbol:	F Xn N	Highly flammable Harmful Dangerous for the environment
R-phrases:	11-38-50/53-65-67	Highly flammable. Irritating to skin. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. Harmful: may cause lung damage if swallowed. Vapours may cause drowsiness and dizziness.
S-phrases:	9-16-29-33-60-61-62	Keep container in a well-ventilated place. Keep away from sources of ignition - No smoking. Do not empty into drains. Take precautionary measures against static discharges. This material and its container must be disposed of as hazardous waste. Avoid release to the environment. Refer to special instructions/Safety data sheets. If swallowed, do not induce vomiting; seek medical advice immediately and show this container or label.
EC-No.:	205-563-8	EC label

Reduced labelling (1999/45/EC, Art. 10, 4)

Symbol:	F Xn N	Highly flammable Harmful Dangerous for the environment
R-phrases:	65	Harmful: may cause lung damage if swallowed.
S-phrases:	62	If swallowed, do not induce vomiting; seek medical advice immediately and show this container or label.

16. Other information

Reason for alteration

Chapter 5: fire-fighting measures.

General update.

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 characterizes the product with regard to the appropriate safety precautions. It does not represent a guarantee of the properties of the product.