

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 16.10.2017

Version 11.10

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

1.1 Product identifier

Catalogue No.	814584
Product name	4-Propylcyclohexanone for synthesis
REACH Registration Number	01-0000015630-78-XXXX
CAS-No.	40649-36-3

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

Identified uses	Chemical for synthesis 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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Catalogue No.	814584
Product name	4-Propylcyclohexanone for synthesis

Skin irritation, Category 2, H315

Chronic aquatic toxicity, Category 3, H412

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

Warning

Hazard statements

H315 Causes skin irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

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

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

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Catalogue No.	814584
Product name	4-Propylcyclohexanone for synthesis

Index-No. 606-057-00-3

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	C ₉ H ₁₆ O (Hill)
Index-No.	606-057-00-3
EC-No.	406-810-4
Molar mass	140,22 g/mol

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
4-N-Propylcyclohexanone (<= 100 %)		
40649-36-3	01-0000015630-78-XXXX	Skin irritation, Category 2, H315 Chronic aquatic toxicity, Category 3, H412

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.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects

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.

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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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.

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

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.

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7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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

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:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

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Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 120 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 898 Butoject® (full contact), KCL 890 Vitoject® (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-(P2)

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.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless

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Odour	weak
Odour Threshold	No information available.
pH	6,0 at 2 g/l 20 °C
Melting point	< -70 °C
Boiling point/boiling range	219 °C at 1.013 hPa
Flash point	90 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	0,23 hPa at 20 °C
Relative vapour density	No information available.
Density	0,91 g/cm ³ at 20 °C
Relative density	No information available.

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Water solubility	1,96 g/l at 20 °C
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Partition coefficient: n-octanol/water	log Pow: 2,62 (experimental) Bioaccumulation is not expected. (own results)
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Auto-ignition temperature	No information available.
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Decomposition temperature	No information available.
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Viscosity, dynamic	No information available.
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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9.2 Other data

Ignition temperature	320 °C Method: DIN 51794
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SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, Nitric acid, acids

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10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 2.000 mg/kg

(own results)

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: Irritations

OECD Test Guideline 404

Causes skin irritation.

Eye irritation

Rabbit

Result: slight irritation

OECD Test Guideline 405

Sensitisation

This information is not available.

Germ cell mutagenicity

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Genotoxicity in vivo

Micronucleus test

Result: negative

(own results)

Genotoxicity in vitro

Ames test

Result: negative

(own results)

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

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

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 Danio rerio (zebra fish): 43 mg/l; 96 h

OECD Test Guideline 203

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Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 33 mg/l; 48 h

OECD Test Guideline 202

12.2 Persistence and degradability

Biodegradability

1,2 %; 28 d

OECD Test Guideline 301D

Not readily biodegradable.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,62

(experimental)

Bioaccumulation is not expected. (own results)

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

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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 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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Sea transport (IMDG)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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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
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Legislation	Not applicable
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Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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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

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).
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National legislation

Storage class	10 - 13
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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.

H315	Causes skin irritation.
H412	Harmful to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

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Labelling

Hazard pictograms



Signal word

Warning

Hazard statements

H227 Combustible liquid.

H315 Causes skin irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

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

P313 Get medical advice/ attention.

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.