MATERIAL SAFETY DATA SHEET
according to the Global Harmonized System

Revision Date 02/04/2013 Version 1.1

SECTION 1.Identification

Product identifier

Product number	814584
Product name	4-Propylcyclohexanone for synthesis

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

Identified uses	Chemical for synthesis

Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
Emergency telephone	613-996-6666 CANUTEC (Canada) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

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.

GHS-Labeling

Hazard pictograms

Signal Word
Warning

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

Precautionary Statements
P273 Avoid release to the environment.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula	$C_9H_{16}O$ (Hill)
CAS-No.	40649-36-3
Molar mass	140.22 g/mol

Hazardous ingredients
Chemical Name (Concentration)
CAS-No.
4-N-Propylcyclohexanone (>= 90 % - <= 100 %)
40649-36-3

SECTION 4. First aid measures
Description of first-aid measures
Inhalation
After inhalation: fresh air.

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

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

Ingestion
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed
irritant effects

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures
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.

Special hazards arising from the substance or mixture

Combustible material, Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapors possible in the event of fire.

Advice for firefighters

Special protective equipment for fire-fighters

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/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into drains.

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.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures
Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection
Safety glasses

Hand protection
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:
protective clothing

Respiratory protection
required when vapors/aerosols are generated.
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	weak
Odor Threshold	No information available.
pH	6.0 at 2 g/l 68 °F (20 °C)
Melting point	< -70 °C
Boiling point/boiling range	426 °F (219 °C) at 1,013 hPa
Flash point	194 °F (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.
Vapor pressure	0.23 hPa at 68 °F (20 °C)

Relative vapor density	No information available.
Relative density	0.91 g/cm³ at 68 °F (20 °C)
Water solubility	1.96 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 2.62 (experimental) Bioaccumulation is not expected (log Pow <1). (own results)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	608 °F (320 °C) Method: DIN 51794

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, Nitric acid, acids

Conditions to avoid

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

Incompatible materials

no information available

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Inhalation, Eye contact, Skin contact

Acute oral toxicity
LD50 rat: > 2,000 mg/kg (own results)

Skin irritation
rabbit
Result: Irritations
OECD Test Guideline 404

Causes skin irritation.

Eye irritation
rabbit
Result: slight irritation
OECD Test Guideline 405

Genotoxicity in vivo
Mutagenicity (mammal cell test): micronucleus.
Result: negative
(own results)

Genotoxicity in vitro
Ames test
Result: negative
(own results)

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish
LC50 Danio rerio (zebra fish): 43 mg/l; 96 h
OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates
EC50 Daphnia magna (Water flea): 33 mg/l; 48 h
OECD Test Guideline 202

Persistence and degradability

Biodegradability
1.2 %; 28 d
OECD Test Guideline 301D
Not readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water
log Pow: 2.62
(experimental)
Bioaccumulation is not expected (log Pow <1). (own results)

Mobility in soil

No information available.

Other adverse effects

Additional ecological information
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)

Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

United States of America

Canada

WHMIS Classification

B3	Combustible Liquid
D2B	Toxic Material Causing Other Toxic Effects

Combustible Liquid, Skin irritant

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

Notification status

TSCA:	Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes. *Ingredients* 4-N-Propylcyclohexanone
DSL:	This product contains one or several components that are not on the Canadian DSL nor NDSL. *Ingredients* 4-N-Propylcyclohexanone

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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.

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.

Revision Date 02/04/2013