

Methylcyclohexane for synthesis

article number: **0752**
Version: **GHS 1.0 en**

date of compilation: 2018-01-22

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

1.1 Product identifier

Identification of the substance	Methylcyclohexane
Article number	0752
Registration number (REACH)	01-2119556887-18-xxxx
Index No	601-018-00-7
EC number	203-624-3
CAS number	108-87-2

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

Identified uses: laboratory chemical

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0

Telefax: +49 (0) 721 - 56 06 149

e-mail: sicherheit@carlroth.de

Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.8D	specific target organ toxicity - single exposure (narcotic effects, drowsiness)	(STOT SE 3)	H336
3.10	aspiration hazard	(Asp. Tox. 1)	H304

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The most important adverse physicochemical, human health and environmental effects

Narcotic effects.

2.2 Label elements

Labelling GHS

Signal word

Danger

Pictograms



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

Precautionary statements

Precautionary statements - prevention

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

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor/physician.
P302+P352	IF ON SKIN: Wash with plenty of water.
P331	Do NOT induce vomiting.
P370+P378	In case of fire: Use sand, carbon dioxide or powder extinguisher to extinguish.

Precautionary statements - storage

P403+P233	Store in a well-ventilated place. Keep container tightly closed.
P403+P235	Store in a well-ventilated place. Keep cool.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H304	May be fatal if swallowed and enters airways.
P331	Do NOT induce vomiting.

2.3 Other hazards

There is no additional information.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Methylcyclohexane
Index No	601-018-00-7
Registration number (REACH)	01-2119556887-18-xxxx
EC number	203-624-3
CAS number	108-87-2
Molecular formula	C ₇ H ₁₄
Molar mass	98.19 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Do NOT induce vomiting. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Aspiration hazard, Irritation, Dizziness, Drowsiness, Narcosis

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours can form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

- **Measures to prevent fire as well as aerosol and dust generation**



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Ground/bond container and receiving equipment.

- **Ventilation requirements**

Use local and general ventilation.

- **Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 – 25 °C.

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Notation	Identifier	TWA [ppm]	TWA [mg/m ³]	STEL [ppm]	STEL [mg/m ³]	Source
AU	methylcyclohexane	108-87-2		WES	400	1,610			WES

Notation

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period unless otherwise specified

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average

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Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	64.3 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	1,355 mg/m ³	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	1.7 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	1.34 µg/l	freshwater	short-term (single instance)
PNEC	0.134 µg/l	marine water	short-term (single instance)
PNEC	273 µg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	3.62 µg/kg	marine sediment	short-term (single instance)
PNEC	36.2 µg/kg	freshwater sediment	short-term (single instance)
PNEC	9.7 µg/kg	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

• type of material

NBR (Nitrile rubber)

• material thickness

0,5 mm

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- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Flame-retardant protective clothing.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C, colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid
Colour	colourless
Odour	characteristic
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	-126.4 °C
Initial boiling point and boiling range	100 – 103 °C
Flash point	-4 °C
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	1.1 vol% (45 g/m ³)
• upper explosion limit (UEL)	6.7 vol%
Explosion limits of dust clouds	not relevant
Vapour pressure	1 kPa at -7.9 °C
Density	0.769 g/cm ³ at 20 °C
Vapour density	3.39 (air = 1)
Bulk density	Not applicable
Relative density	Information on this property is not available.

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Solubility(ies)

Water solubility 14 mg/l at 25 °C

Partition coefficient

n-octanol/water (log KOW) 4.13 (ECHA)

Soil organic carbon/water (log KOC) 2.37 (ECHA)

Auto-ignition temperature 260 °C

Decomposition temperature no data available

Viscosity

• dynamic viscosity 0.679 mPa s at 20 °C

Explosive properties Shall not be classified as explosive

Oxidising properties none

9.2 Other information

Surface tension 23.29 mN/m (25 °C)

Refractive index 1.423

SECTION 10: Stability and reactivity

10.1 Reactivity

Risk of ignition. Vapours can form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: Strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Shall not be classified as acutely toxic.

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Exposure route	Endpoint	Value	Species	Source
oral	LD50	2,250 mg/kg	mouse	
dermal	LD50	>2,000 mg/kg	rabbit	

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

- **Specific target organ toxicity - single exposure**

May cause drowsiness or dizziness.

- **Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

May be fatal if swallowed and enters airways.

Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

data are not available

- **If in eyes**

data are not available

- **If inhaled**

fatigue, narcosis

- **If on skin**

causes skin irritation

Other information

None

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

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Endpoint	Value	Species	Source	Exposure time
LC50	>13.4 mg/l	rainbow trout (<i>Oncorhynchus mykiss</i>)		96 h
EC50	10 – 30 mg/l	<i>Pseudokirchneriella subcapitata</i>		72 h

12.2 Process of degradability

Theoretical Oxygen Demand: 3.422 mg/mg
 Theoretical Carbon Dioxide: 3.137 mg/mg

Process	Degradation rate	Time
biotic/abiotic	0 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) 4.13
 BCF >95 – <321 (ECHA)

12.4 Mobility in soil

Henry's law constant 34,300 Pa m³/mol at 25 °C
 The Organic Carbon normalised adsorption coefficient 2.37

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

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Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.


13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1	UN number	2296
14.2	UN proper shipping name	METHYLCYCLOHEXANE
	Hazardous ingredients	Methylcyclohexane
14.3	Transport hazard class(es)	
	Class	3 (flammable liquids)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	hazardous to the aquatic environment
14.6	Special precautions for user	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7	Transport in bulk according to Annex II of MARPOL and the IBC Code	
	The cargo is not intended to be carried in bulk.	
14.8	Information for each of the UN Model Regulations	
	• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)	
	UN number	2296
	Proper shipping name	METHYLCYCLOHEXANE
	Particulars in the transport document	UN2296, METHYLCYCLOHEXANE, 3, II, (D/E), environmentally hazardous
	Class	3
	Classification code	F1
	Packing group	II
	Danger label(s)	3 + "fish and tree"

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Environmental hazards	yes (hazardous to the aquatic environment)
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	33
Emergency Action Code	3YE

• International Maritime Dangerous Goods Code (IMDG)

UN number	2296
Proper shipping name	METHYLCYCLOHEXANE
Particulars in the shipper's declaration	UN2296, METHYLCYCLOHEXANE, 3, II, -4°C c.c., MARINE POLLUTANT
Class	3
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	3 + "fish and tree"



Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-E, S-D
Stowage category	B

• International Civil Aviation Organization (ICAO-IATA/DGR)

UN number	2296
Proper shipping name	Methylcyclohexane
Particulars in the shipper's declaration	UN2296, Methylcyclohexane, 3, II
Class	3
Environmental hazards	yes (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	3

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Exempted quantities (EQ)

E2

Limited quantities (LQ)

1 L

SECTION 15: Regulatory information

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

National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	short-term exposure limit
TWA	time-weighted average
vPvB	very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne conatminants

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Key literature references and sources for data

- UN Recommendations on the Transport of Dangerous Good
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
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

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.