

SAFETY DATA SHEET



n-Heptanoic acid
10520

Version / Revision 3
Supersedes Version 2.01

Revision Date 05-May-2020
Issuing date 15-May-2020

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

1.1. Product identifier

Identification of the substance/preparation

n-Heptanoic acid

Chemical Name Heptanoic acid
CAS-No 111-14-8
EC No. 203-838-7
Registration number (REACH) 01-2119463877-21

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

Identified uses Transported isolated intermediate (1907/2006)
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking Identification **OQ Chemicals Corporation**
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA

Product Information Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number +65 3158 1198 (available 24/7)
000800 100 7479 (for domestic shipments only)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Acute inhalation toxicity Category 4, H332
Skin corrosion/irritation Category 1B, H314
Serious eye damage/eye irritation Category 1, H318
Target Organ Systemic Toxicant - Single exposure Category 3, H335

Additional information

For full text of Hazard- and EU Hazard-statements see SECTION 16.

2.2. Label elements

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Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).

Hazard pictograms



Signal word

Danger

Hazard statements

H332: Harmful if inhaled.
H314: Causes severe skin burns and eye damage.
H335: May cause respiratory irritation.

Precautionary statements

P260: Do not breathe gas/mist/vapours.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310: Immediately call a POISON CENTER/doctor.
P403 + P233: Store in a well ventilated place. Keep container tightly closed.

2.3. Other hazards

Components of the product may be absorbed into the body by inhalation

PBT and vPvB assessment This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACH-No	1272/2008/EC	Concentration (%)
Heptanoic acid	111-14-8	01-2119463877-21	Acute Tox. 4; H332 Skin Corr. 1B; H314 Eye Dam. 1; H318 STOT SE 3; H335	> 98,5

For full text of Hazard- and EU Hazard-statements see SECTION 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Keep at rest. Aerate with fresh air. Symptoms of poisoning may develop many hours after exposure. Call a physician immediately.

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Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Immediate medical attention is required.

Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion

Call a physician immediately. Do not induce vomiting without medical advice.

4.2. Most important symptoms and effects, both acute and delayed

Main symptoms

cough, headache, nausea, shortness of breath, vomiting, convulsions.

Special hazard

Lung irritation, Lung oedema.

4.3. Indication of any immediate medical attention and special treatment needed

General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. If ingested, flush stomach and compensate acidosis.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

foam, dry chemical, carbon dioxide (CO₂), water spray

Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO₂)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapours are heavier than air and may spread along floors

5.3. Advice for firefighters

Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting

Cool containers / tanks with water spray. Water run-off and vapor cloud may be corrosive. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.

For emergency responders: Personal protection see section 8.

6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant).

6.3. Methods and material for containment and cleaning up

Methods for containment

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

bases
amines

7.2. Conditions for safe storage, including any incompatibilities

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material.

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Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Keep at temperatures between 0 and 38 °C (32 and 100 °F).

Temperature class

T3

7.3. Specific end use(s)

Transported isolated intermediate (1907/2006)

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits India

No exposure limits established.

8.2. Exposure controls

Appropriate Engineering controls

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	nitrile rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0.55 mm
Break through time	> 480 min
Suitable material	polyvinylchloride / nitrile rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0.9 mm
Break through time	> 480 min

Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

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Equipment should conform to EN 166

Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	liquid
Colour	colourless
Odour	pungent
Odour threshold	0,6 - 10,4 ppm
pH	4,8 @ 20 °C (68 °F)
Melting point/range	-8 °C
Boiling point/range	223 °C @ 1013 hPa
Flash point	117 °C
Method	DIN EN ISO 3679
Evaporation rate	No data available
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	1,09 Vol %
Upper explosion limit	10,1 Vol %

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
0,013	0,0013	< 0,001	20	68	
0,2	0,02	< 0,001	50	122	

Vapour density 4,5 (Air = 1) @ 20 °C (68 °F)

Relative density

Values	@ °C	@ °F	Method
0,92	20	68	

Solubility 2 - 5 g/l @ 25 °C, in water

log Pow 2,54 (calculated), KOW WIN

Autoignition temperature 275 °C

Method EU A.15

Decomposition temperature No data available

Viscosity 3,4 mPa*s @ 30 °C

Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

9.2. Other information

Molecular weight	130,19
Molecular formula	C7 H14 O2
log Koc	1,143

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Refractive index 1,422 @ 20 °C

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerisation does not occur.

10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

10.5. Incompatible materials

bases, amines.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Ingestion, Inhalation, Eye contact, Skin contact

Acute toxicity				
Heptanoic acid (111-14-8)				
Routes of Exposure	Endpoint	Values	Species	Method
Inhalative	LC50	> 4,6 mg/l (4h)	rat, male/female	OECD 403

Heptanoic acid, CAS: 111-14-8

Assessment

The available data lead to the classification given in section 2

Dermal acute toxicity data were not determined, because of the corrosive properties of the substance

For acute oral toxicity, no data are available

Irritation and corrosion				
Heptanoic acid (111-14-8)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	

Heptanoic acid, CAS: 111-14-8

Assessment

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The available data lead to the classification given in section 2
Available skin corrosion data suffice for classification of eye corrosion without further testing
For respiratory irritation, no data are available

Sensitization				
Heptanoic acid (111-14-8)				
Target Organ Effects	Species	Evaluation	Method	
Skin	guinea pig	not sensitizing	OECD 406	

Heptanoic acid, CAS: 111-14-8

Assessment

Based on available data, the classification criteria are not met for:
Skin sensitization
For respiratory sensitization, no data are available

Heptanoic acid, CAS: 111-14-8

Assessment

Due to lack of data, a classification is not possible for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Heptanoic acid (111-14-8)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Developmental Toxicity	NOAEL 1000 mg/kg/d	rat		OECD 414, Oral	Maternal toxicity
Developmental Toxicity	NOAEL 1000 mg/kg/d	rat		OECD 414, Oral	Teratogenicity

Heptanoic acid, CAS: 111-14-8

CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

Evaluation

In vitro tests did not show mutagenic effects

Heptanoic acid, CAS: 111-14-8

Main symptoms

cough, headache, nausea, shortness of breath, vomiting, convulsions.

Target Organ Systemic Toxicant - Single exposure

The available data lead to the classification given in section 2

Target Organ Systemic Toxicant - Repeated exposure

Due to lack of data, a classification is not possible for:
STOT RE

Aspiration toxicity

no data available

Other adverse effects

Components of the product may be absorbed into the body by inhalation.

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:

<http://echa.europa.eu/information-on-chemicals/registered-substances>.

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SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Heptanoic acid (111-14-8)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 860 mg/l	OECD 202
Pimephales promelas (fathead minnow)	96h	LC50: > 92 mg/l	OECD 203
green algae	96h	EC50: 122,7 mg/l (Growth rate)	ECOSAR
Pseudomonas putida	17 h	EC50: > 1000 mg/l (Growth inhibition)	DIN 38412, part 8

12.2. Persistence and degradability

Heptanoic acid, CAS: 111-14-8

Biodegradation

98,7 % (11 d), Sewage, domestic, non-adapted, aerobic, OECD 301 A / ISO 7827.

12.3. Bioaccumulative potential

Heptanoic acid (111-14-8)		
Type	Result	Method
log Pow	2,54	KOW WIN, calculated

12.4. Mobility in soil

Heptanoic acid (111-14-8)		
Type	Result	Method
Adsorption/Desorption	log Koc: 1,143	

12.5. Results of PBT and vPvB assessment

Heptanoic acid, CAS: 111-14-8

PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

12.6. Other adverse effects

Heptanoic acid, CAS: 111-14-8

No data available

Note

Avoid release to the environment.

SECTION 13: Disposal considerations

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13.1. Waste treatment methods

Product Information

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Hazardous waste according to European Waste Catalogue (EWC)

Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

SECTION 14: Transport information

ICAO-TI / IATA-DGR

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (n-Heptanoic acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (n-Heptanoic acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	F-A, S-B
14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code	
Product name	n-Heptanoic acid
Ship type	3
Pollution category	Z

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI

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Classification	Skin Corr. 1B; H314
Hazard pictograms	GHS05 Corrosion
Signal word	Danger
Hazard statements	H314

International Inventories

Heptanoic acid, CAS: 111-14-8

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2038387 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-18284 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)
TCSI (TW)

National regulatory information India

Hazardous Chemicals, Schedule 2: Threshold Quantities at an Isolated Storage
not listed

Hazardous Chemicals, Schedule 3: Threshold Quantities in an Industrial Installation
not listed

For details and further information please refer to the original regulation.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3

H314: Causes severe skin burns and eye damage.

H318: Causes serious eye damage.

H332: Harmful if inhaled.

H335: May cause respiratory irritation.

Abbreviations

A table of terms and abbreviations can be found under the following link:

http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

Training advice

For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet

Information contained in this safety data sheet is based on OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet

Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the OQ homepage (www.chemicals.oq.com).

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The annex is not required because the substance is registered as an intermediate under REACH

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End of Safety Data Sheet