

SAFETY DATA SHEET



n-Heptanoic acid
10520

Version / Revision 2
Supersedes Version 1.00***

Revision Date 13-Jan-2021
Issuing date 13-Jan-2021

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

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

Use of the Substance /
Preparation Intermediate.
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 +44 (0) 1235 239 670 (UK) available 24/7***
NCEC +1 202 464 2554
Local emergency telephone
number +61 2 8014 4558 (Australia)
18000 74234 (Australia toll-free number)
+64 9 929 1483 (New Zealand)
0800 446 881 (New Zealand toll-free number)
+65 3158 1195 (Sri Lanka)
007 803 011 0293 (Indonesia toll-free number)
+60 3 6207 4347 (Malaysia)
001 800 120 666 751 (Thailand toll-free number)
+65 3158 1200 (Bangladesh)
+63 2 8231 2149 (Philippines)
+84 28 4458 2388 (Vietnam)
+65 3165 2217 (Singapore)
available 24/7

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SECTION 2: Hazards identification

Europe

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

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)***

USA

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2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).***

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***

OSHA Specified Hazards Not applicable.

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).***

Hazard symbol(s) ***



Signal word

Danger***

Hazard statements

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

Precautionary statements

Prevention

P280: Wear protective gloves/protective clothing/eye protection/face protection.
P260: Do not breathe gas/mist/vapours.
P271: Use only outdoors or in a well ventilated area.
P264: Wash hands thoroughly after handling.***

Response

P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P363: Wash contaminated clothing before reuse.
P310: Immediately call a POISON CENTER/doctor.***

Storage

P403 + P233: Store in a well ventilated place. Keep container tightly closed.
P405: Store locked up.***

Disposal

P501: Dispose of contents/container in accordance with local regulation.***

2.3. Other hazards

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

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

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.

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

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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.

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

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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.

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 European Union

No exposure limits established***

Exposure limits Germany

No exposure limits established.

Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.***

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.

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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.

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.

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

Skin and body protection

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

Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (dust). Equipment should conform to NIOSH, EN or other applicable national standards.

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

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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
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

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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

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	negative	OECD 471	In vitro study

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		typhimurium		(Ames)	
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>.

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

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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

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

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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 ***
EmS 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

ADR/RID

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 ***
ADR Tunnel restriction code (E)
Classification Code C3
Hazard Number 80

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI

Heptanoic acid***, CAS: 111-14-8

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

DI 2012/18/EU (Seveso III) ***

Category not subject***

DI 1999/13/EC (VOC Guideline)

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Component	Status
Heptanoic acid*** CAS: 111-14-8	not subject***

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)***

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).

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

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

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End of Safety Data Sheet