SAFETY DATA SHEET

n-Heptanoic acid
10520

Version / Revision	3.01	**Revision Date**	27-Jan-2022
Supersedes Version	2.01	**Issuing date**	27-Jan-2022

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

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	> 95,5

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.

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.

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.

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.

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 @ 1013 hPa***
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	OECD 104***
0,2	0,02	< 0,001	50	122	OECD 104***

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

Relative density

Values	@ °C	@ °F	Method
0,918***	20	68	

Solubility	1,96 - 5,32 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
Method	dynamic***
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	1,2 calculated***
Dissociation constant	pKa 4,75 @ 20 °C (68 °F) (calculated)***
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	
Respiratory tract***	rat***	irritating***	OECD 403***	4h***

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

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

Subacute, subchronic and prolonged toxicity				
Heptanoic acid (111-14-8)				
Type	Dose	Species	Method	
Subacute toxicity***	NOAEL: 1750 mg/kg/d***	rat, male/female***	OECD 407***	Oral***
Subacute toxicity***	LOAEL: 3500 mg/kg/d***	rat, male/female***	OECD 407***	Oral***
Subchronic toxicity***	NOAEL: 1000 mg/kg/d***	rat, male/female***	OECD 408***	Oral***

Heptanoic acid*, CAS: 111-14-8**
Assessment
Based on available data, the classification criteria are not met 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
Mutagenicity***		human lymphocytes***	negative***	OECD 473 (Chromosomal Aberration)***	In vitro study***
Mutagenicity***		mouse lymphoma cells***	negative***	OECD 476 (Mammalian Gene Mutation)***	In vitro study***
Developmental Toxicity***	NOAEL 300 mg/kg/d***	rabbit***		OECD 414, Oral***	Maternal toxicity***
Developmental	NOAEL > 1000	rabbit***		OECD 414,	Fetal toxicity,

Toxicity***	mg/kg/d***			Oral***	Embryotoxicity***
Reproductive toxicity***	NOAEL < 200 mg/kg/d***	rat, parental, female***		OECD 421***	Maternal toxicity***
Reproductive toxicity***	NOAEL 1000 mg/kg/d***	rat, 1. Generation, male/female***		OECD 421***	

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
Based on available data, the classification criteria are not met for:
Reproductive toxicity
Developmental toxicity
Mutagenicity***

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
Based on available data, the classification criteria are not met 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	72h***	EC50: 61,2 mg/l (Growth rate)	OECD 201***
Pseudomonas putida	17 h	EC50: > 1000 mg/l (Growth inhibition)	DIN 38412, part 8
Daphnia magna (Water flea)***	48 h***	EC50: 72 mg/l***	OECD 203***
Oryzias latipes (Medaka)***	96 h***	LC50: 74,8 mg/l***	OECD 203***

Long term toxicity
Heptanoic acid (111-14-8)

Type	Species	Dose	Method	
Reproductive toxicity***	Daphnia magna (Water flea)***	NOEC: 40 mg/l (21d)***	OECD 211***	
Aquatic toxicity***	Pseudokirchneriella subcapitata***	NOEC: 46 mg/l (3d) Growth rate***	OECD 201***	

Terrestrial toxicity				
Heptanoic acid (111-14-8)				
Species	Exposure time	Dose	Type	Method
Eisenia fetida***	56 d***	NOEC: 10 mg/kg soil dw***	Reproduction***	OECD 222***
Eisenia fetida***	28 d***	NOEC: > 32 mg/kg soil dw***	Mortality***	OECD 222***
Beta vulgaris (Sugar beet)***	21 d***	NOEC: 7,6 mg/kg soil dw***	Growth***	OECD 208***
Brassica rapa (Turnip)***	21 d***	EC10: 1,2 mg/kg soil dw***	Growth***	OECD 208***
Lactuca sativa (Lettuce)***	21 d***	EC10: 27,7 mg/kg soil dw***	Growth***	OECD 208***
Lolium perenne (Ryegrass)***	21 d***	NOEC: 7,6 mg/kg soil dw***	Growth***	OECD 208***
Soil microorganism***	28 d***	NOEC: 300 mg/kg soil dw***	Nitrogen transformation***	OECD 216***

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.

Abiotic Degradation		
Heptanoic acid (111-14-8)		
Type	Result	Method
Hydrolysis***	not expected***	
Photolysis***	not expected***	

12.3. Bioaccumulative potential

Heptanoic acid (111-14-8)		
Type	Result	Method
log Pow	2,54	KOW WIN, calculated
BCF***	No data available***	

12.4. Mobility in soil

Heptanoic acid (111-14-8)		
Type	Result	Method
Adsorption/Desorption	log Koc: 1,2	calculated***
Surface tension***	no data available***	
Distribution to environmental	no data available***	

compartments***		

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

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
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

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

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).
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.

End of Safety Data Sheet