Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU

N-Octyl-2-pyrrolidone ≥ 99%, for synthesis

article number: **0358**
Version: **1.0 en**

date of compilation: 2017-07-25

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

1.1 Product identifier

Identification of the substance	**N-Octyl-2-pyrrolidone**
Article number	0358
Registration number (REACH)	01-0000015335-74-xxxx
Index No	613-098-00-0
EC number	403-700-8
CAS number	2687-94-7

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

Identified uses:

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 according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS

Section	Hazard class	Hazard class and category	Hazard statement
3.2	skin corrosion/irritation	(Skin Corr. 1B)	H314
3.3	serious eye damage/eye irritation	(Eye Dam. 1)	H318
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 2)	H411

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word **Danger**

Pictograms

Hazard statements

H314	Causes severe skin burns and eye damage
H411	Toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P273	Avoid release to the environment.
P280	Wear protective gloves/eye protection.

Precautionary statements - response

P303+P361+P353	IF ON SKIN (or hair): take off immediately all contaminated clothing. Rinse skin with water/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.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)

H314	Causes severe skin burns and eye damage.
P273	Avoid release to the environment.
P280	Wear protective gloves/eye protection.
P303+P361+P353	IF ON SKIN (or hair): take off immediately all contaminated clothing. Rinse skin with water/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.

2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	N-Octyl-2-pyrrolidone
Index No	613-098-00-0
Registration number (REACH)	01-0000015335-74-xxxx
EC number	403-700-8
CAS number	2687-94-7
Molecular formula	$C_{12}H_{23}NO$
Molar mass	197,3 $^{g}/_{mol}$

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Take off immediately all contaminated clothing.

Following inhalation

Remove person to fresh air and keep comfortable for breathing. If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions.

Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure.

Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

Following ingestion

Rinse mouth immediately and drink plenty of water. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects). Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Irritation, Corrosion, Breathing difficulties, Gastric perforation, Risk of serious damage to eyes

4.3 Indication of any immediate medical attention and special treatment needed

none

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 may form explosive mixtures with air.

Hazardous combustion products

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

5.3 Advice for firefighters

Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Do not breathe vapour/spray. Avoid contact with skin, eyes and clothes.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provide adequate ventilation. Handle and open container with care. Clear contaminated areas thoroughly.

Advice on general occupational hygiene

Wash hands before breaks and after work.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

• 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)

Data are not available.

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	17,45 mg/m³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	2,5 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0,091 mg/l	freshwater	short-term (single instance)
PNEC	0,009 mg/l	marine water	short-term (single instance)
PNEC	170 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	3,08 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0,308 mg/kg	marine sediment	short-term (single instance)
PNEC	0,248 mg/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. Wear face protection.

Skin protection

• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. 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

Butyl caoutchouc (butyl rubber)

• material thickness

0,7mm

• 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.

Respiratory protection

Respiratory protection necessary at: Aerosol or mist formation. Type: A-P2 (combined filters against particles and organic gases and vapours, colour code: Brown/White).

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 (fluid)
Colour	colourless - light yellow
Odour	like: amine
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	7 – 10
Melting point/freezing point	-26 °C
Initial boiling point and boiling range	297 – 307 °C
Flash point	142 °C (DIN 51758)
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)

Explosive limits	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	not relevant
Vapour pressure	0,0008 hPa at 20 °C 0,02 hPa at 55 °C
Density	0,92 $^{g}/_{cm^3}$ at 20 °C
Vapour density	This information is not available.
Bulk density	Not applicable
Relative density	Information on this property is not available.
Solubility(ies)	
Water solubility	~ 1 $^{g}/_{l}$ at 20 °C
Partition coefficient	
n-octanol/water (log KOW)	This information is not available.
Auto-ignition temperature	225 °C - (DIN 51794)
Decomposition temperature	475 °C
Viscosity	
• kinematic viscosity	9,1 $^{mm^2}/_{s}$ at 20 °C
• dynamic viscosity	8,4 mPa s at 20 °C
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

9.2 Other information

Temperature class (EU, acc. to ATEX)	T3 (Maximum permissible surface temperature on the equipment: 200°C)

SECTION 10: Stability and reactivity

10.1 Reactivity

In case of warming: 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: Acids, Strong oxidiser

10.4 Conditions to avoid
Keep away from heat. Decompostion takes place from temperatures above: 475 °C.

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.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	>2.200 $^{mg}/_{kg}$	rat	ECHA
dermal	LD50	>4.000 $^{mg}/_{kg}$	rat	ECHA

Skin corrosion/irritation
Causes severe burns.

Serious eye damage/eye irritation
Causes serious eye damage.

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

• Specific target organ toxicity - repeated exposure
Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard
Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed
If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

• If in eyes
causes burns, Causes serious eye damage, risk of blindness

• If inhaled
Irritation to respiratory tract, cough, breathing difficulties

• If on skin
causes severe burns, causes poorly healing wounds

Other information
None

SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	>12,8 – <44,8 $^{mg}/_{l}$	fish	ECHA	96 h
EC50	7,59 $^{mg}/_{l}$	aquatic invertebrates	ECHA	48 h
ErC50	19 $^{mg}/_{l}$	algae	ECHA	72 h

Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

Endpoint	Value	Species	Source	Exposure time
EC50	460 $^{mg}/_{l}$	microorganisms	ECHA	30 min
LOEC	2,8 $^{mg}/_{l}$	fish	ECHA	35 d
NOEC	0,91 $^{mg}/_{l}$	fish	ECHA	35 d
growth (EbCx) 10%	170 $^{mg}/_{l}$	microorganisms	ECHA	30 min

12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,959 $^{mg}/_{mg}$
Theoretical Oxygen Demand: 2,676 $^{mg}/_{mg}$
Theoretical Carbon Dioxide: 2,676 $^{mg}/_{mg}$

12.3 Bioaccumulative potential

The substance fulfils the very bioaccumulative criterion. Data are not available.

12.4 Mobility in soil

Data are not available.

Henry's law constant 0,023 $^{Pa\ m^3}/_{mol}$ at 25 °C

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. Avoid release to the environment. Refer to special instructions/safety data sheets.

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	**3267**
14.2	UN proper shipping name	**CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S.**
	Hazardous ingredients	N-Octyl-2-pyrrolidone
14.3	Transport hazard class(es)	
	Class	8 (corrosive substances)
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.

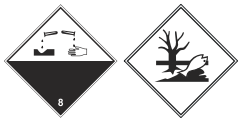
14.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

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)

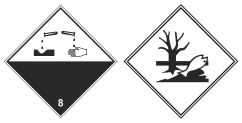
UN number	3267
Proper shipping name	CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S.
Particulars in the transport document	UN3267, CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S., (N-Octyl-2-pyrrolidone), 8, II, (E), environmentally hazardous
Class	8
Classification code	C7
Packing group	II
Danger label(s)	8 + "fish and tree"



Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	E
Hazard identification No	80
Emergency Action Code	2X

• International Maritime Dangerous Goods Code (IMDG)

UN number	3267
Proper shipping name	CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S.
Particulars in the shipper's declaration	UN3267, CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S., (N-Octyl-2-pyrrolidone), 8, II, MARINE POLLUTANT
Class	8
Marine pollutant	yes (hazardous to the aquatic environment)
Packing group	II
Danger label(s)	8 + "fish and tree"



Special provisions (SP)	274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-A, S-B
Stowage category	B
Segregation group	18 - Alkalis

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

UN number	3267
Proper shipping name	Corrosive liquid, basic, organic, n.o.s.
Particulars in the shipper's declaration	UN3267, Corrosive liquid, basic, organic, n.o.s., (N-Octyl-2-pyrrolidone), 8, II
Class	8
Environmental hazards	yes (hazardous to the aquatic environment)
Packing group	II

Danger label(s)	8

Special provisions (SP)	A3, 274
Excepted quantities (EQ)	E2
Limited quantities (LQ)	0,5 L

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

• Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)
Not listed.

• Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)
Not listed.

• Regulation 850/2004/EC on persistent organic pollutants (POP)
Not listed.

• Restrictions according to REACH, Annex XVII

Name of substance	CAS No	Wt%	Type of registration	No
N-Octyl-2-pyrrolidone		100	1907/2006/EC annex XVII	3

• List of substances subject to authorisation (REACH, Annex XIV)
not listed

• Seveso Directive

2012/18/EU (Seveso III)

No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200	500	57)

Notation
57) Hazardous to the Aquatic Environment in category Chronic 2

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II
not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- DSL/NDSL (Canada)
- REACH (Europe)
- Toxic Substance Control Act (TSCA)

15.2 Chemical Safety Assessment

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

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)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
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

Abbr.	Descriptions of used abbreviations
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)
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- 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
H314	causes severe skin burns and eye damage
H318	causes serious eye damage
H411	toxic to aquatic life with long lasting effects

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.