SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006, as amended by Commission Regulation (EU) 2020/878

Version 6.12
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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name	:	n-Octane for synthesis
Product Number	:	8.06910
Catalogue No.	:	806910
Brand	:	Millipore
Index-No.	:	601-009-00-8
REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration or the annual tonnage does not require a registration.
CAS-No.	:	111-65-9

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

Identified uses	:	Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company	:	Merck Pty Ltd. 259 Davidson Road, Corner Peddie Road WADEVILLE, GERMISTON 1428 SOUTH AFRICA
Telephone	:	+27 (0) 8600 63725
Fax	:	+27 (0) 860 522 329

1.4 Emergency telephone number

Emergency Phone #	:	0-800-983-611 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquids, Category 2	H225: Highly flammable liquid and vapour.
Skin irritation, Category 2	H315: Causes skin irritation.
Specific target organ toxicity -	H336: May cause drowsiness or dizziness.

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single exposure, Category 3, Central nervous system	
Aspiration hazard, Category 1	H304: May be fatal if swallowed and enters airways.
Short-term (acute) aquatic hazard, Category 1	H400: Very toxic to aquatic life.
Long-term (chronic) aquatic hazard, Category 1	H410: Very toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms :

Signal word : Danger

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.
H410	Very toxic to aquatic life with long lasting effects.

Precautionary statements :

Prevention:

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P331	Do NOT induce vomiting.

Reduced Labelling (<= 125 ml)

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Hazard pictograms :

Signal word	Danger
Hazard Statements H304	May be fatal if swallowed and enters airways.
Precautionary Statements P301 + P310 P331	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Do NOT induce vomiting.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Index-No. : 601-009-00-8

EC-No. : 203-892-1

Components

Chemical name	CAS-No. EC-No.	Concentration (% w/w)	M-Factor, SCL, ATE
n-octane	111-65-9 203-892-1	>= 90 - <= 100	M-Factor (Acute aquatic toxicity): 1

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice : Show this safety data sheet to the doctor in

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attendance.

If inhaled	:	After inhalation: fresh air. Call in physician.
In case of skin contact	:	In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
In case of eye contact	:	After eye contact: rinse out with plenty of water. Remove contact lenses.
If swallowed	:	After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media	:	Carbon dioxide (CO2) Foam Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Specific hazards during fire fighting	:	Combustible. Pay attention to flashback. Vapours are heavier than air and may spread along floors. Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.
Hazardous combustion products	:	Carbon oxides

5.3 Advice for firefighters

Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
Further information	:	Remove container from danger zone and cool with water.

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Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Personal precautions : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Keep away from heat and sources of ignition.
Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Environmental precautions : Do not let product enter drains.
Risk of explosion.

6.3 Methods and material for containment and cleaning up

Methods for cleaning up : Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal considerations see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Temperature class : T3

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of

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ignition.

Storage class (TRGS 510)	:	3, Flammable liquids
Further information on storage stability	:	Store below +30°C.
Recommended storage temperature	:	Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure Limits

8.2 Exposure controls

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0,4 mm
Protective index	:	Full contact
Manufacturer	:	Camatril® (KCL 730 / Aldrich Z677442, Size M)

Material	:	Nitrile rubber
Break through time	:	30 min
Glove thickness	:	0,11 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 741 Dermatril® L
Remarks	:	This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Skin and body protection	:	Flame retardant antistatic protective clothing.
Respiratory protection	:	required when vapours/aerosols are generated. Our recommendations on filtering respiratory

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protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type:	:	Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Advice	:	Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	:	liquid (20 °C, 1.013 hPa)
Color	:	colourless
Odor	:	characteristic
Melting point/ range	:	-57 °C
Boiling point/boiling range	:	125 - 126 °C (1.013 hPa)
Flammability	:	No data available
Upper explosion limit / Upper flammability limit	:	Upper flammability limit 6,5 %(V)
Lower explosion limit / Lower flammability limit	:	Lower flammability limit 0,96 %(V)
Flash point	:	13 °C Method: closed cup
Autoignition temperature	:	220 °C
Decomposition temperature	:	No data available
pH	:	No data available

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Viscosity		
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	0,8 mm2/s (20 °C)
Flow time	:	No data available
Solubility(ies)		
Water solubility	:	ca. 0,007 g/l (20 °C)
Partition coefficient: n-octanol/water	:	log Pow: 5,15
Vapor pressure	:	14,7 hPa (20,0 °C)
Relative density	:	No data available
Density	:	0,70 g/cm3 (20 °C)
Relative vapour density	:	No data available

9.2 Other information

Explosives	:	Not classified as explosive.
Oxidizing properties	:	none
Burning rate	:	No data available
Self-ignition	:	220 °C
Evaporation rate	:	No data available
Molecular weight	:	114,26 g/mol

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

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10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Hazardous reactions : Violent reactions possible with:

Strong oxidizing agents
various plastics

10.4 Conditions to avoid

Conditions to avoid : Warming.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - > 5.000 mg/kg
(OECD Test Guideline 401)
Remarks: The value is given in analogy to the following substances: isooctane
LC50 Inhalation - Rat - male and female - 4 h - > 24,88 mg/l - vapour

(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)
Remarks: The value is given in analogy to the following substances: isooctane

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin. - 24 h
(OECD Test Guideline 404)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: isooctane
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: isooctane

Respiratory or skin sensitization
Maximisation Test - Guinea pig
Result: negative
(OECD Test Guideline 406)
Remarks: (in analogy to similar products)

Germ cell mutagenicity

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Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Remarks: The value is given in analogy to the following substances: n-heptaneTest Type: Chromosome aberration test in vitro
Test system: rat hepatocytes
Method: OECD Test Guideline 473
Result: negative
Remarks: The value is given in analogy to the following substances: n-heptaneTest Type: In vitro mammalian cell gene mutation test
Test system: human lymphoblastoid cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Remarks: The value is given in analogy to the following substances: isooctane**Carcinogenicity**
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause drowsiness or dizziness. - Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

RTECS: RG8400000
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Vomiting, Central nervous system depression, narcosis
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

After uptake of large quantities:

Headache
Dizziness
Nausea

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Vomiting
agitation
somnolence
Drowsiness
Unconsciousness
respiratory arrest

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Components:

n-octane:

Toxicity to fish	:	LC50 (Oryzias latipes): 0,42 mg/l End point: mortality Exposure time: 96,0 h Remarks: (Lit.)
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 0,38 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Remarks: (ECOTOX Database)
Toxicity to algae/aquatic plants	:	NOEC (Pseudokirchneriella subcapitata (microalgae)): 5,8 mg/l End point: Growth inhibition Exposure time: 72 h Remarks: (Lit.)
M-Factor (Acute aquatic toxicity)	:	1
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	:	NOEC: 0,17 mg/l Exposure time: 21 d Species: Daphnia magna (Water flea) Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes Remarks: (in analogy to similar products)

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Ecotoxicology Assessment

Acute aquatic toxicity	:	Very toxic to aquatic life.
Chronic aquatic toxicity	:	Very toxic to aquatic life with long lasting effects.

12.2 Persistence and degradability

Components:

n-octane:

Biodegradability	:	Test Type: aerobic Concentration: 3,3 mg/l Result: Readily biodegradable. Biodegradation: 70,3 % Exposure time: 10 d Remarks: (ECHA)
ThOD	:	3.500 mg/g Remarks: (Lit.)

12.3 Bioaccumulative potential

Components:

n-octane:

Partition coefficient: n-octanol/water	:	log Pow: 5,15

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

Product:

Assessment	:	This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment	:	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

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SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product	:	Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

14.1 UN number or ID number

ADR	:	UN 1262
IMDG	:	UN 1262
IATA	:	UN 1262

14.2 UN proper shipping name

ADR	:	OCTANES
IMDG	:	OCTANES
IATA	:	Octanes

14.3 Transport hazard class(es)

		Class	Subsidiary risks
ADR	:	3	
IMDG	:	3	
IATA	:	3	

14.4 Packing group

ADR

Packing group	:	II
Classification Code	:	F1
Hazard Identification Number	:	33
Labels	:	3
Tunnel restriction code	:	(D/E)

IMDG

Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-E

IATA (Cargo)

Packing instruction (cargo aircraft)	:	364
Packing instruction (LQ)	:	Y341
Packing group	:	II
Labels	:	Class 3 - Flammable liquids

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IATA_P (Passenger)

Packing instruction (passenger aircraft)	:	353
Packing instruction (LQ)	:	Y341
Packing group	:	II
Labels	:	Class 3 - Flammable liquids

14.5 Environmental hazards

ADR

Environmentally hazardous	:	yes

IMDG

Marine pollutant	:	yes

14.6 Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

SECTION 15: Regulatory information

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

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)	:	Conditions of restriction for the following entries should be considered: Number on list 3 Number on list 40 This substance/mixture shall not be used in aerosol dispensers intended for supply to the general public for entertainment and decorative purposes. Number on list 75 If you intend to use this product as tattoo ink, please contact your vendor.
REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59).	:	Not applicable
Regulation (EU) No 2024/590 on substances that deplete the ozone layer	:	Not applicable
Regulation (EU) 2019/1021 on persistent organic	:	Not applicable

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pollutants (recast)

REACH - List of substances subject to authorisation (Annex XIV)	:	Not applicable
Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.	E1	ENVIRONMENTAL HAZARDS
	P5c	FLAMMABLE LIQUIDS

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

Full text of other abbreviations

Aquatic Acute	:	Short-term (acute) aquatic hazard
Aquatic Chronic	:	Long-term (chronic) aquatic hazard
Asp. Tox.	:	Aspiration hazard
Flam. Liq.	:	Flammable liquids
Skin Irrit.	:	Skin irritation
STOT SE	:	Specific target organ toxicity - single exposure

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CLP - Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECHA - European Chemicals Agency; EC-Number - European Community number; ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC -

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New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; SVHC - Substance of Very High Concern; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TRGS - Technical Rule for Hazardous Substances; TSCA - Toxic Substances Control Act (United States); UN - United Nations; vPvB - Very Persistent and Very Bioaccumulative

Further information

Other information : The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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REG_EU / EN

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