

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.02.2015

Version 5.2

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

1.1 Product identifier

Catalogue No.	808469
Product name	2-Undecanone for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	112-12-9

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number

Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

N Dangerous for the environment R50/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word
Warning

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Product name 2-Undecanone for synthesis

Hazard statements

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

CAS-No. 112-12-9

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ (CH ₂) ₈ COCH ₃	C ₁₁ H ₂₂ O (Hill)
EC-No.	203-937-5	
Molar mass	170,29 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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2-undecanone, n- (<= 100 %)		
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112-12-9	*)	
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Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
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2-undecanone, n- (<= 100 %)	
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112-12-9	N, Dangerous for the environment; R50/53
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For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

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SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water.

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed

The following applies to ketones in general: when vapours/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

4.3 Indication of any immediate medical attention and special treatment needed

No information 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

Combustible material, Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Special protective equipment for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

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Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 mm
Break through time:	> 240 min

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The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 730 Camatril® -Velours (full contact), KCL 720 Camapren® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment
protective clothing

Respiratory protection
required when vapours/aerosols are generated.
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds
The entrepreneur 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
Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	yellow
Odour	pleasant
Odour Threshold	No information available.
pH	No information available.
Melting point	11 - 13 °C
Boiling point/boiling range	228 °C at 1.013 hPa
Flash point	96 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	0,01 hPa at 20 °C

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Relative vapour density	5,87
Density	0,83 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C practically insoluble
Partition coefficient: n-octanol/water	log Pow: 4,09 (experimental) A remarkable bioaccumulation potential is expected (log Po/w >3). (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	> 400 °C
Viscosity, dynamic	1,61 mPa.s at 30 °C
Explosive properties	No information available.
Oxidizing properties	No information available.

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, Strong bases

10.4 Conditions to avoid

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 5.000 mg/kg (RTECS)

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

LD50 Rabbit: > 5.000 mg/kg (RTECS)

Skin irritation

This information is not available.

Eye irritation

This information is not available.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Other information

The following applies to ketones in general: when vapours/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 1,5 mg/l; 96 h (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 0,54 mg/l; 48 h (ECOTOX Database)

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Product name 2-Undecanone for synthesis

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 4,09

(experimental)

A remarkable bioaccumulation potential is expected (log Po/w >3). (Lit.)

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number UN 3082

14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (METHYL NONYL KETONE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous yes

14.6 Special precautions for user yes

Tunnel restriction code E

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 3082

14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (METHYL NONYL KETONE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous yes

14.6 Special precautions for user no

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Sea transport (IMDG)

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Catalogue No. 808469
Product name 2-Undecanone for synthesis

14.1 UN number UN 3082
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (METHYL NONYL KETONE)
14.3 Class 9
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
EmS F-A S-F
Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9
14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC
Legislation Dangerous for the environment
9a
Quantity 1: 100 t
Quantity 2: 200 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 10 - 13

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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SECTION 16. Other information

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

H400 Very toxic to aquatic life.
H410 Very toxic to aquatic life with long lasting effects.

Full text of R-phrases referred to under sections 2 and 3

R50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Warning

Hazard statements

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Labelling (67/548/EEC or 1999/45/EC)

Symbol(s)  N Dangerous for the environment

R-phrases 50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

S-phrases 61 Avoid release to the environment. Refer to special instructions/ Safety data sheets.

EC-No. 203-937-5

Reduced labelling (≤125 ml)

Symbol(s)  N Dangerous for the environment

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.