

PRODUCT: 2-METHYLUDECANAL
Aroma chemical

Version: 5
revised: 15.06.2015
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1 IDENTIFICATION OF THE SUBSTANCE AND OF THE COMPANY/ UNDERTAKING

1.1 Product identifier: 2-Methylundecanal
CAS-No.: 110-41-8, EC-No.: 203-765-0
REACH registration number: 01-2119969443-29-0003
Product no.: 0101061000
FEMA-No.: 2749

1.2 Relevant identified uses of the substance: Aroma chemical
Uses advised against: no data available

1.3 Details of the supplier of the safety data sheet:

Miltitz Aromatics GmbH
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1.4 Emergency telephone number:
+49 361 730 730

2 HAZARDS IDENTIFICATION

2.1 Classification according to the classification rules in Regulation (EC) Nr. 1272/2008

Hazard Class/es:	Hazard Class/es and Hazard Category/ies-Code:	Hazard Statement/s:
Skin corrosion/irritation	Skin Irrit. 2	H315: Causes skin irritation
Respiratory/skin sensitisation	Skin Sens. 1	H317: May cause an allergic skin reaction.
Hazardous to the aquatic environment	Aquatic Acute 1 Aquatic Chronic 1	H400: Very toxic to aquatic life. H410: Very toxic to aquatic life with long lasting effects

2.2 Label elements according to Regulation (EC) Nr. 1272/2008

Hazard pictogram/s:

Signal word:

Warning



GHS07



GHS09

Hazard Statement/s: The Hazard Statement/s are contain in the section 2.1.

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Precautionary Statement/s:

Prevention:	P261	Avoid breathing gas/mist/vapours/spray.
	P264	Wash the skin thoroughly after handling.
	P272	Contaminated work clothing should not be allowed out of the workplace.
	P273	Avoid release to the environment.
	P280	Wear protective gloves/protective clothing/eye protection/face protection.
Response:	P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
	P333 + P313	If skin irritation or rash occurs: Get medical advice/attention.
	P362 + P364	Take off contaminated clothing and wash it before reuse.
	P391	Collect spillage.
Disposal:	P501	Dispose of contents to a waste management service provider according to the local law and regulations.

2.3 Other hazards: Not known.
The properties of the substance do not filling the criteria for the PBT or vPvB classification.

3 COMPOSITION/INFORMATION ON INGREDIENTS

Min. 96% 2-Methylundecanal,
CAS-No.: 110-41-8, EC-No.: 203-765-0

4 FIRST AID MEASURES

4.1 Description of first aid measures:

In case of inhalation: Move affected person into fresh air, keep warm and allow to rest.
In case of skin (or hair) contact: Wash immediately with water and soap. Remove contaminated, saturated clothing immediately.
In case of eye contact: Flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist if problems persist.
In case of ingestion: Do not induce vomiting. Rinse mouth immediately and drink plenty of water and seek medical advice.
If there is a risk of loss of consciousness, place and transport affected person in the recovery position. No administration in cases of unconsciousness or cramps.

4.2 Most important symptoms and effects, both acute and delayed:
Causes skin irritation and may cause sensitisation by skin contact.

4.3 Indication of any immediate medical attention and special treatment needed:
Symptomatically treatment.

5 FIREFIGHTING MEASURES

5.1 Extinguishing media:

Suitable extinguishing media: Dry extinguishing powder; carbon dioxide (CO₂); foam.
Unsuitable extinguishing media: Full water jet.

5.2 Special hazards arising from the substance:

In case of fire may be liberated: carbon dioxide (CO₂), carbon monoxide (CO), toxic pyrolysis products.

5.3 Advice for fire-fighters:

Wear a self-contained breathing apparatus and chemical protective clothing.
Dispose of fire debris and contaminated extinguishing water in accordance with official regulations.
Keep containers cool by spraying with water if exposed to fire.

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6 ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures:**
for non-emergency personnel: Provide adequate ventilation.
Avoid contact with skin, eyes and clothing.
Wear protective gloves/protective clothing/eye protection/face protection.
Remove all sources of ignition, avoid heat and sparks.
for emergency responders: In case of large amounts wear a self-contained breathing apparatus and chemical protective clothing. No further precautions.
- 6.2 Environmental precautions:** Do not allow to enter drains/surface water/ground-water.
Do not allow to enter into soil/subsoil.
In case of entry into waterways, soil or drains, inform the responsible authorities.
Treat the recovered material as prescribed in the section on waste disposal.
- 6.3 Methods and material for containment and cleaning up:**
For large amount: dike spillage. Pump off product.
For residues: Pick up with suitable absorbent material
Suitable material for taking up: universal binder.
- 6.4 Reference to other sections:** See the sections 8 und 13 of the safety data sheet to.

7 HANDLING AND STORAGE

- 7.1 Precautions for safe handling:**
Use only in well-ventilated areas.
Avoid inhalation, skin contact, eye contact.
When using do not eat, drink or smoke.
Wash hands before breaks and after work.
Remove contaminated clothing and protective equipment before entering eating areas.
Keep working clothes separately. Wash thoroughly after handling.
Only use the material in places where open light, fire and other sources of ignition can be kept away.
- 7.2 Conditions for safe storage, including any incompatibilities**
Store in the original container under protective gas (nitrogen).
Keep container tightly closed. Keep in a cool, dry, well-ventilated place protected from direct sunlight.
Floor should be solvent-resistant, closed, sealed and not adsorbent.
- 7.3 Specific end use(s)**
Aroma chemical.

8 EXPOSURE CONTROLS/PERSONAL PROTECTION

- 8.1 Control parameters**
2-Methylundecanal CAS-No.: 110-41-8
To date, no national critical limit values exist.

DNEL:		for workers	for general population
Inhalation, systemic:	Long-term:	25.2 mg/m ³	3.1 mg/m ³
Dermal, systemic:	Long-term:	7 mg/kg	3.5 mg/kg
Dermal, local:	Long-term:	1.67 mg/cm ²	0.83 mg/cm ²
Oral, systemic:	Long-term:		3.5 mg/kg

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8.2 Exposure controls

8.2.1 Engineering controls: See section 7.1

8.2.2 Personal protective equipment:

Eye / face protection:

Suitable eye protection: Eye glasses with side protection (according to EN 166).

Skin protection:

- Hand protection:

- By long-term hand contact:

Suitable gloves type (recommended protective index 6, corresponding >480 min of permeation time according to EN 374):

Butyl caoutchouc (butyl rubber), 0.7 mm coating thickness

- By short-term hand contact

Suitable gloves type (recommended at least protective index 2, corresponding >30 min of permeation time according to EN 374):

CR (polychloroprene, chloroprene rubber) 0.5 mm coating thickness

Supplementary note:

The specifications are based on literature and information of glove manufacturer or are derived from similar substances by analogy. Due to many conditions (e.g. temperature) it must be considered, that the practical usage of a chemical-protective glove in practice may be much shorter than the determined permeation time.

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.

- Other: Suitable protective clothing:

For the protection against direct skin contact, body protective clothing is essential (in addition to the usual working clothes).

Respiratory protection:

Respiratory protection necessary if insufficient ventilation.

Self-contained respirator (DIN EN 133) or container device with compressed air (DIN EN 137).

Filtering device (full mask or mouthpiece) with filter A (EN 14387).

8.2.3 Environmental exposure controls:

Do not allow to enter drains/surface water/ground-water.

Do not allow to enter into soil/subsoil.

9 PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Property	Value	Unit of measurement	method
Appearance:	colourless liquid		
Odour:	fruity-fatty, reminiscent of orange and amber		
Odour threshold:	not known		
pH-value:	not applicable		
Melting point / freezing point:	< -50	°C	OECD 102
Boiling point:	231	°C (1013 hPa)	OECD 103
Flash point:	68.5	°C	EU A.9
Evaporation rate:	not known		
Explosive limits:	not explosive		
Vapour pressure:	0.85	Pa (at 20 °C)	OECD 104
Vapour density:	not known		

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9.1	Relative density (D _{20/4}):	0.826 – 0.829	g/cm ³ (20 °C)	
Con-	Solubility/ies, in water:	1.3	mg/l (at 20 °C)	OECD 105
tinu-	in org. solvents:	miscible with most organic solvents		
ation	Partition coefficient			
	n-octanol/water (log K _{ow}):	4.9	(at 35 °C)	OECD 117
	Self-Ignition temperature:	205	°C (at 1013 hPa)	EU A.15
	Decomposition temperature:	no decomposition until boiling point		
	Viscosity:	3.3	mm ² /s (at 20 °C)	OECD 114
	Explosive properties:	not explosive	expert statement	
	Oxidising properties:	not oxidising	expert statement	

Other information

Surface tension: 58.1 mN/m (at 19.6 °C) (90% saturated solution)
The substance is considered to be surface active.

10 STABILITY AND REACTIVITY

10.1 Reactivity

No hazardous reactions known.

10.2 Chemical stability

No hazardous reaction if stored and handled as prescribed.

10.3 Possibility of hazardous reactions

No hazardous reaction if stored and handled as prescribed.

10.4 Conditions to avoid

No hazardous decomposition if stored and handled as prescribed.

10.5 Incompatible materials

No hazardous reactions known.

10.6 Hazardous decomposition products

No hazardous decomposition products if stored and handled as prescribed.

11 TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

		Test according to
Acute toxicity: LD ₅₀ /oral/rat:	> 5 000 mg/kg	(Huntingdon, Baltimore 1971a)
LD ₅₀ /dermal/rat:	> 8 280 mg/kg	(Huntingdon, Baltimore 1971b)
Inhalation:	no data available	
Skin corrosion / irritation:	irritant (rabbit)	(Huntingdon, Baltimore 1971c)
Serious eye damage / irritation:	not irritating (rabbit)	(Frey.Tox 1999)
Respiratory or skin sensitisation:	skin sensitising	(Unilever 2000, LLNA-Test [mouse], OECD 429)
Mutagenicity: Bacterial Reverse Mutation Assay		
(AMES-Test, OECD 471)		negative
Gene mutation, in vitro (OECD 476)		negative without metabolic activation
		positive with metabolic activation
		Data from a test using analogue substance Nonanal
Chromosome aberration,		negative for Chromosome aberration
in vitro (OECD 473)		positive for SCE induction
		Data from a test using analogue substance Nonanal

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- 11.1 Con- tinu- ation** **Mutagenicity:** Micronucleus test, in vivo (OECD 474) **Test according to** negative
Germ cell mutagenicity: No experimental indications of genotoxicity in-vitro exist.
Carcinogenicity: no data available
Reproductive toxicity/rat/oral: Screening test: **NOAEL: 300 mg/kg, LOAEL: 1500 mg/kg**
Data from a test using analogue substance undec-10-enal
Data from a test using analogue substance 2,6-Dimethylhept-5-enal
One-generation study: **NOAEL: 200 mg/kg, LOAEL: 1500 mg/kg**
Data from a test using analogue substance Heptanoic acid
STOT-single exposure: no data available
STOT-repeated exposure/rat: **NOAEL: 20 000 ppm (= 1409.7 mg/kg), 90 d in diet, OECD 408**
Data from a test using analogue substance Dodecanal
Aspiration hazard: no data available
- 11.2** **Most important symptoms and effects, both acute and delayed:**
Causes skin irritation and may cause sensitisation by skin contact.

12 ECOLOGICAL INFORMATION

- 12.1 Toxicity:**
- **Fish toxicity:** **LC₅₀: 0.35 mg/l (96 h) (Oncorhynchus mykiss [rainbow trout])** **OECD 203**
 - **Daphnia toxicity:** **EC₅₀: 0.21 mg/l (48 h) (Daphnia magna [Big water flea])** **OECD 202**
 - **Algae toxicity:** **ErC₅₀: 0.18 mg/l (72h) (growth rate, Pseudokirchnerella subcapitata)** **OECD 201**
(NOEC: 0.089 mg/l [72h])

- 12.2 Persistence and degradability:**
Readily biodegradable
Degradation: 68 % after 22 d (O₂ consumption, OECD 301 F, Manometric Respiration Test)
Degradation: 68 % after 28 d (CO₂ evolution, OECD 301 B, CO₂ Evolution Test)

- 12.3 Bioaccumulative potential:**
Based on the n-octanol/water partition coefficient the accumulation in organisms can be expected.
A BCF of ≤ 778 L/kg can be calculated*, which support the potential for a bioaccumulation.
* The readily biodegradability status and an in vitro study showing that linear aldehydes are rapidly metabolised by trout liver S9 fractions, support a reduced BCF compared to estimates based only on log Kow. A regression QSAR corroborated with analogue data and models that take biotransformation into account all give BCF estimates range from 34 to 778 L/kg.

- 12.4 Mobility in soil:**
The adsorption coefficient was determined with $\lg K_{oc} = 3.6$ ($K_{oc} = 3981$) in accordance to OECD 121.
Based on the test results the substance is not considered to be highly adsorptive indicating that soil and sediment are not expected to be the main target components for exposure assessment.

- 12.5 Results of PBT and vPvB assessment:**
The properties of the substance do not filling the criteria for the PBT or vPvB classification.

- 12.6 Other adverse effects**
Impact on sewage plants
Technically correct releases of minimal concentrations to adapted biological sewage plants will not disturb the biodegradability of activated sludge.

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13 DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Dispose of waste according to applicable local, state, and federal regulations.

Waste code: 07 06 00

Waste name: wastes from the manufacture, formulation, supply and use (MFSU) of acids of fats, grease, soaps, detergents, disinfectants and cosmetics.

Appropriate disposal / packaging: Contaminated packing must be completely emptied and can be re-used following proper cleaning.

14 TRANSPORT INFORMATION

14.1 UN number: UN 3082

14.2 UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (2-Methylundecanal)

14.3 Transport hazard class(es): 9

14.4 Packing group: III

14.5 Environmental hazards: Marine pollutant: yes (acute and chronic toxicity, category 1)

14.6 Special precautions for user: Do not allow to enter drains/surface water/ground-water.
Do not allow to enter into soil/subsoil.

14.7 Transport in IBC possible: IBC-Code: IBC03

14.8 Further specific data for the different kinds of transport:

LAND TRANSPORT
(ADR/RID):

Classification code: M6

Hazardous number: 90

Tunnel code: (-)

MARINE TRANSPORT
(IMDG/GGV SEE):

EmS-Code: F-A, S-F

Stowage/segregation:

Category A

Marine pollutant: yes

AIR TRANSPORT (ICAO-TI / IATA-
DGR):

IATA packing instruction:

passenger aircraft: 964 Qty./ Pckg.: 450 ltr.

cargo aircraft: 964 Qty./ Pckg.: 450 lit.

15 REGULATORY INFORMATION

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

There are no specific regulations/legislation.

National regulations:

Water hazard class (WGK): 2 Water-endangering

Classification according to VwVwS (Germany, 17th May 1999), Annex 3
using R-phrases as stated in this Safety Data Sheet.

However the substance is officially classified into the WGK 1 (weakly water-endangering) according to VwVwS (Germany, 17th May 1999), Annex 3 (VwVwS Code Number: 3316). It is to expect that this classification will be changed due to the REACH registration data.

15.2 Chemical safety assessment

A safety assessment was made in connection with the REACH registration procedure.

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16 OTHER INFORMATION

■ Data changed in the version 5 in comparison to the version 4, dated 23.03.2015, are marked by a ■ in the left column.

Literature:

- REGULATION (EC) No 1907/2006 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
- Commission Regulation (EU) 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)
- REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006

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. This description of the product does not represent a guarantee for properties of the product.

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