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trans-Hexen-2-al ≥98,5 %, for synthesis

article number: **3757** Version: **GHS 2.0 en** Replaces version of: 2021-05-19 Version: (GHS 1)

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

1.1 Product identifier

Identification of the substance

Article number

CAS number

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6728-26-3

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

Relevant identified uses:

Uses advised against:

Laboratory chemical Laboratory and analytical use

Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

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 Department Health, Safety and Environment sheet:

e-mail (competent person):

sicherheit@carlroth.de

1.4 Emergency telephone number

| Name | Street | Postal code/city | Telephone | Website |
|--|-----------------|-------------------------|-----------|---------|
| NSW Poisons Information Centre Childrens Hospital | Hawkesbury Road | 2145 West- mead, NSW | 131126 | |

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

| Section | Hazard class | Cat- egory | Hazard class and category | Hazard statement |
|---------|-------------------------|---------------|---------------------------|---------------------|
| 2.6 | Flammable liquid | 3 | Flam. Liq. 3 | H226 |
| 3.10 | Acute toxicity (oral) | 4 | Acute Tox. 4 | H302 |
| 3.1D | Acute toxicity (dermal) | 3 | Acute Tox. 3 | H311 |
| 3.4S | Skin sensitisation | 1 | Skin Sens. 1 | H317 |

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word Danger

Pictograms

GHS02, GHS06



Hazard statements

| H226 H302 | Flammable liquid and vapour Harmful if swallowed |
|--------------|---|
| H311 | Toxic in contact with skin |
| H317 | May cause an allergic skin reaction |
| | |

Precautionary statements

Precautionary statements - prevention

| P210 | Keep away from heat/sparks/open flames/hot surfaces No smoking |
|------|--|
| P261 | Avoid breathing dust/fume/gas/mist/vapours/spray |
| P280 | Wear protective gloves/protective clothing |

Precautionary statements - response

| P302+P352 | IF ON SKIN: Wash with plenty of soap and water |
|-----------|---|
| P312 | Call a POISON CENTER or doctor/physician if you feel unwell |
| P370+P378 | In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction |

Precautionary statements - storage

P403+P235 Store in a well-ventilated place. Keep cool

Precautionary statements - disposal

Dispose of contents/container to industrial combustion plant

2.3 Other hazards

P501

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

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3.1

SECTION 3: Composition/information on ingredients

| Substances | |
|-------------------|-------------------------------------|
| Name of substance | trans-Hexen-2-al |
| Molecular formula | C ₆ H ₁₀ O |
| Molar mass | 98.14 ^g / _{mol} |
| CAS No | 6728-26-3 |

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

Following inhalation

Provide fresh air.

Following skin contact

After contact with skin, wash immediately with plenty of water. In case of skin reactions, consult a physician.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Allergic reactions

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 firefighting measures to the fire surroundings! water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

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5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapourair mixture.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. 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

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

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

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (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

Provision of sufficient ventilation. Handle and open container with care. Clear contaminated areas thoroughly.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

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Advice on general occupational hygiene

Thorough skin-cleansing after handling the product. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Store locked up. Ground/bond container and receiving equipment.

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)

This information is not available.

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side 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. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effect-ive layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

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• type of material

NBR (Nitrile rubber)

• material thickness

>0,11 mm

• 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 (against organic gases and vapours with a boiling point of > 65 $^{\circ}$ C, colour code: Brown).

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

| Physical state | liquid |
|---|---|
| Colour | light yellow |
| Odour | characteristic |
| Melting point/freezing point | 146.5 °C (ECHA) |
| Boiling point or initial boiling point and boiling range | 147 °C at 1,013 hPa (ECHA) |
| Flammability | flammable liquid in accordance with GHS criteria |
| Lower and upper explosion limit | not determined |
| Flash point | 38 °C at 1,013 hPa (ECHA) |
| Auto-ignition temperature | 218 °C at 102 kPa (ECHA) |
| Decomposition temperature | not relevant |
| pH (value) | not determined |
| Kinematic viscosity | not determined |
| <u>Solubility(ies)</u> Water solubility | 5.261 ^g / _l at 25 °C (ECHA) |
| Partition coefficient Partition coefficient n-octanol/water (log value): | 1.58 (25 °C) (ECHA) |

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| | Vapour pressure | 0.63 kPa at 25 °C |
|-----|---|---|
| | Density and/or relative density | |
| | Density | 0.849 ^g / _{cm³} at 22 °C (ECHA) |
| | Relative vapour density | 3.39 (air = 1) |
| | Particle characteristics | not relevant (liquid) |
| | Other safety parameters | |
| | Oxidising properties | none |
| 9.2 | Other information | |
| | Information with regard to physical hazard classes: | There is no additional information. |
| | Other safety characteristics: | There is no additional information. |

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition.

If heated

Risk of ignition. Vapours may 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: strong oxidiser, Strong alkali, Reducing agents

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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

Classification acc. to GHS

Acute toxicity

Harmful if swallowed. Toxic in contact with skin.

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| Acute toxicity | | | | | |
|----------------|----------|-----------------------------------|---------|--------|--------|
| Exposure route | Endpoint | Value | Species | Method | Source |
| oral | LD50 | 685 ^{mg} / _{kg} | mouse | | |
| oral | LD50 | 780 ^{mg} / _{kg} | rat | | |
| dermal | LD50 | 600 ^{mg} / _{kg} | rabbit | | |

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

May cause an allergic skin reaction.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified 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

diarrhoea, vomiting, abdominal pain

• If in eyes

slightly irritant

• If inhaled

Data are not available.

• If on skin

Irritating to skin, May produce an allergic reaction, pruritis, localised redness

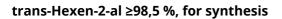
Other information

Health effects are not known.

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

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SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.608 ^{mg}/_{mg} Theoretical Carbon Dioxide: 2.691 ^{mg}/_{mg}

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| n-octanol/water (log KOW) | 1.58 (25 °C) (ECHA) |
|---------------------------|---------------------|
|---------------------------|---------------------|

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

12.7 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.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

Relevant provisions relating to waste(Basel Convention)

Properties of waste which render it hazardous

H3 Flammable liquids

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. Non-contaminated packages may be recycled.



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SECTION 14: Transport information

| 14.1 | UN number | |
|------|--|--|
| | UN RTDG | UN 1988 |
| | IMDG-Code | UN 1988 |
| | ICAO-TI | UN 1988 |
| 14.2 | UN proper shipping name | |
| | UN RTDG | ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. |
| | IMDG-Code | ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. |
| | ICAO-TI | Aldehydes, flammable, toxic, n.o.s. |
| | Technical name | Trans-Hexen-2-al |
| 14.3 | Transport hazard class(es) | |
| | UN RTDG | 3 (6.1) |
| | IMDG-Code | 3 (6.1) |
| | ICAO-TI | 3 (6.1) |
| 14.4 | Packing group | |
| | UN RTDG | III |
| | IMDG-Code | III |
| | ICAO-TI | III |
| 14.5 | Environmental hazards | non-environmentally hazardous acc. to the dan- gerous goods regulations |
| 14.6 | Special precautions for user There is no additional information. | |
| 14.7 | Transport in bulk according to IMO instrument The cargo is not intended to be carried in bulk. | 5 |
| 14.8 | Information for each of the UN Model Regulation | ons |
| | Transport informationNational regulationsAdd | itional information(UN RTDG) |
| | UN number | 1988 |
| | Class | 3 |
| | Subsidiary risk(s) | 6.1 |
| | Packing group | III |
| | Danger label(s) | 3+6.1 |
| | | |

223, 274 UN RTDG





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| Excepted quantities (EQ) | E1 UN RTDG | | | |
|---|---|--|--|--|
| Limited quantities (LQ) | 5 L UN RTDG | | | |
| Emergency Action Code | 3W | | | |
| International Maritime Dangerous Goods Code (IMDG) - Additional information | | | | |
| Proper shipping name | ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. | | | |
| Particulars in the shipper's declaration | UN1988, ALDEHYDES, FLAMMABLE, TOXIC, N.O.S., (trans-Hexen-2-al), 3 (6.1), III, 38°C c.c. | | | |
| Marine pollutant | - | | | |
| Danger label(s) | 3+6.1 | | | |
| | | | | |
| Special provisions (SP) | 223, 274 | | | |
| Excepted quantities (EQ) | E1 | | | |
| Limited quantities (LQ) | 5 L | | | |
| EmS | F-E, S-D | | | |
| Stowage category | A | | | |
| International Civil Aviation Organization (IC | AO-IATA/DGR) - Additional information | | | |
| Proper shipping name | Aldehydes, flammable, toxic, n.o.s. | | | |
| Particulars in the shipper's declaration | UN1988, Aldehydes, flammable, toxic, n.o.s., (trans-Hexen-2-al), 3 (6.1), III | | | |
| Danger label(s) | 3+6.1 | | | |
| | | | | |
| Special provisions (SP) | A3 | | | |
| Excepted quantities (EQ) | E1 | | | |
| Limited quantities (LQ) | 2 L | | | |
| | | | | |

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS) Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

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National inventories

| Country | Inventory | Status |
|---------|------------|------------------------------|
| AU | AIIC | substance is listed |
| CA | DSL | substance is listed |
| CN | IECSC | substance is listed |
| EU | ECSI | substance is listed |
| EU | REACH Reg. | substance is listed |
| JP | CSCL-ENCS | substance is listed |
| KR | KECI | substance is listed |
| MX | INSQ | substance is listed |
| NZ | NZIoC | substance is listed |
| PH | PICCS | substance is listed |
| TW | TCSI | substance is listed |
| US | TSCA | substance is listed (ACTIVE) |
| VN | NCI | substance is listed |

Legend

15.2 Chemical Safety Assessment

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

SECTION 16: Other information

Indication of changes (revised safety data sheet)

| Section | Former entry (text/value) | Actual entry (text/value) | Safety- relev- ant |
|---------|---------------------------|---|--------------------------|
| 2.3 | | Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%. | yes |
| 14.8 | | Emergency Action Code: 3W | yes |
| 15.1 | | Other information: Directive 94/33/EC on the protection of young people at work. Observe employment restric- tions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers. | yes |
| 15.1 | | National inventories: change in the listing (table) | yes |

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Abbreviations and acronyms

| Abbr. | Descriptions of used abbreviations |
|-----------|--|
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| ED | Endocrine disruptor |
| 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 Na- tions |
| IATA | International Air Transport Association |
| IATA/DGR | Dangerous Goods Regulations (DGR) for the air transport (IATA) |
| ICAO | International Civil Aviation Organization |
| ICAO-TI | Technical instructions for the safe transport of dangerous goods by air |
| IMDG | International Maritime Dangerous Goods Code |
| IMDG-Code | International Maritime Dangerous Goods Code |
| LD50 | Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval |
| NLP | No-Longer Polymer |
| PBT | Persistent, Bioaccumulative and Toxic |
| UN RTDG | UN Recommendations on the Transport of Dangerous Good |
| vPvB | Very Persistent and very Bioaccumulative |

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

| Code | Text |
|------|--------------------------------------|
| H226 | Flammable liquid and vapour. |
| H302 | Harmful if swallowed. |
| H311 | Toxic in contact with skin. |
| H317 | May cause an allergic skin reaction. |

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.