

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Trade name : TRANS-2-HEXENAL
Revision date : 27.05.2015
Print date : 27-05-2015

Version (Revision) : 2.1.0 (2.0.1)

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

1.1 Product identifier

TRANS-2-HEXENAL (W01055)
trans-hex-2-enal ; CAS No. : 6728-26-3 ; EC No. : 229-778-1

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

Relevant identified uses

Flavour and fragrance ingredient. Fragrance ingredient which may be used in fragrance compounds according to the current legislation and IFRA rules. Reserved for industrial and professional use.

Uses advised against

-

1.3 Details of the supplier of the safety data sheet

Supplier (manufacturer/importer/only representative/downstream user/distributor)

PFW Aroma Chemicals B.V.

Street : Veemweg 29-31

Postal code/city : NL - 3371 MT Barneveld

Telephone : +31 342 40 77 00

Telefax : +31 342 40 77 20

Information contact : pfw@pfw.nl

1.4 Emergency telephone number

+31 342 40 77 93

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Aquatic Chronic 2 ; H411 - Hazardous to the aquatic environment : Category 2 ; Toxic to aquatic life with long lasting effects.

Acute Tox. 3 ; H311 - Acute toxicity (dermal) : Category 3 ; Toxic in contact with skin.

Acute Tox. 4 ; H302 - Acute toxicity (oral) : Category 4 ; Harmful if swallowed.

Flam. Liq. 3 ; H226 - Flammable liquids : Category 3 ; Flammable liquid and vapour.

Skin Sens. 1 ; H317 - Skin sensitisation : Category 1B ; May cause an allergic skin reaction.

Hazard classes and hazard categories

Flam. Liq. 3 · Acute Tox. 4 (Oral) · Acute Tox. 3 (Dermal) · Skin Irrit. 3 · Skin Sens. 1B · Aquatic Acute 2 · Aquatic Chronic 2

Classification according to Directive 67/548/EEC or 1999/45/EC

Flammable. · Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. · May cause sensitization by skin contact. · Harmful in contact with skin and if swallowed.

R 10 · N ; R 51/53 · R 43 · Xn ; R 21/22

2.2 Label elements

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

Hazard pictograms

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Flame (GHS02) · Skull and crossbones (GHS06) · Environment (GHS09)

Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.
H311 Toxic in contact with skin.
H302 Harmful if swallowed.
H317 May cause an allergic skin reaction.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P235 Keep cool.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/container to a chemical waste treatment facility or recycling plant.

2.3 Other hazards

None

SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name : trans-hex-2-enal

EC No. : 229-778-1

CAS No. : 6728-26-3

Purity : ≥ 99 % [mass]

Synonyms

IUPAC : Hex-2-enal

INCI : TRANS-2-HEXENAL

SECTION 4: First aid measures

4.1 Description of first aid measures

General information

Medical examination necessary even merely on suspicion of intoxication. Remove victim out of the danger area. Put victim at rest, cover with a blanket and keep warm. Do not leave affected person unattended. If unconscious place in recovery position and seek medical advice.

In case of inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial

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respiration.

In case of skin contact

Change contaminated, saturated clothing. Water After contact with skin, wash immediately with plenty of water and soap. Call a physician immediately. Do not wash with: Solvents/Thinner

After 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.

After ingestion

Rinse mouth thoroughly with water. Call a physician in any case! Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

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

alcohol resistant foam. Extinguishing powder.

Unsuitable extinguishing media

Strong water jet. Water mist.

5.2 Special hazards arising from the substance or mixture

Hazardous combustion products

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

5.3 Advice for firefighters

Do not inhale explosion and combustion gases. Use water spray jet to protect personnel and to cool endangered containers. Do not allow run-off from fire-fighting to enter drains or water courses. Toxic to aquatic life. May cause long lasting harmful effects to aquatic life.

Special protective equipment for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Special danger of slipping by leaking/spilling product. Keep away from sources of ignition. - No smoking. Do not breathe gas/fumes/vapour/spray. Provide adequate ventilation. Remove persons to safety. See protective measures under point 7 and 8.

6.2 Environmental precautions

Ensure all waste water is collected and treated via a waste water treatment plant. In case of entry into waterways, soil or drains, inform the responsible authorities. Toxic to aquatic life. May cause long lasting harmful effects to aquatic life.

6.3 Methods and material for containment and cleaning up

Suitable material for taking up: Sand, Kieselguhr, Universal binder, Sawdust. Collect in closed and suitable containers for disposal.

6.4 Reference to other sections

See protective measures under point 7 and 8.

SECTION 7: Handling and storage

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7.1 Precautions for safe handling

Provide adequate ventilation as well as local exhaust at critical locations. When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work. All work processes must always be designed so that the following is as low as possible: eye contact, skin contact, inhalation of vapours or spray/mists. In case of entry into waterways, soil or drains, inform the responsible authorities. Wear personal protection equipment (see chapter 8). Use explosion-proof machinery, apparatus, ventilation facilities, tools etc. Use only antistatically equipped (spark-free) tools. Take precautionary measures against static discharge. Keep away from sources of ignition. - No smoking. Vapours can form explosive mixtures with air.

7.2 Conditions for safe storage, including any incompatibilities

Technical measures and storage conditions

Ensure adequate ventilation of the storage area. Keep/Store only in original container. Use isolated drainage to prevent discharge to soil. Restrict access to stockrooms. Take precautionary measures against static discharge. Keep away from sources of ignition. - No smoking. Keep the packing dry and well sealed to prevent contamination and absorption of humidity. Never use pressure to empty container.

Hints on joint storage

Keep away from oxidising agent, acid and alkali.

Storage class : 3

Storage class (TRGS 510) : 3

7.3 Specific end use(s)

None

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

To date, no national critical limit values exist.

8.2 Exposure controls

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work.

Appropriate engineering controls

Provide adequate ventilation as well as local exhaust at critical locations. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Personal protection equipment

Eye/face protection

Eye glasses with side protection

Skin protection

Hand protection

Gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. Breakthrough times and swelling properties of the material must be taken into consideration.

Suitable material : Butyl caoutchouc (butyl rubber)

Breakthrough time (maximum wearing time) : >240 min.

Thickness of the glove material : 1.00 mm.

Recommended glove articles : Butyl Plus/R0,5

Body protection

Overall

Respiratory protection

Respiratory protection necessary at: exceeding exposure limit values insufficient ventilation insufficient exhaust Handling larger quantities. Container device with compressed air (DIN EN 137) / Filtering device (full mask or

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mouthpiece) with filter: Filter types:A, B, E, K. Class 1: Maximum permitted contaminant concentration in inhaled air = 1000 mL/m³ (0.1 % by vol.); class 2: maximum permitted contaminant concentration in inhaled air = 5000 mL/m³ (0.5 % by vol.); class 3: maximum permitted contaminant concentration in inhaled air = 10000 mL/m³ (1.0 % by vol.)

Environmental exposure controls

Send to a hazardous waste incinerator facility under observation of official regulations.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Odour threshold in air : No data available

Safety relevant basis data

Physical state :			liquid	
Colour :			colourless to pale yellow	
Odour :			fruity green	
Boiling temperature/boiling range :	(1013 hPa)		159 °C	
Freezing point :		<	-20 °C	
Flash point (Closed Cup) :			35 °C	DIN EN 51578
Auto-ignition temperature :			235 °C	
Decomposition temperature			No data available	
Lower explosion limit :			No data available	
Upper explosion limit :			No data available	
Explosive properties :			none	
Vapour pressure :	(20 °C)	ca.	4,55 hPa	
Evaporation rate (n-butylacetate = 1) :			0,7	
Surface tension (20°C)	(20 °C)		No data available	
Relative density (water = 1) :	(20 °C)		0,841 - 0,848	
Density :	(20 °C)		0,842 - 0,85 g/cm ³	
Water solubility :			slightly soluble (0.1-100 mg/l)	
pH value :			No data available	
Log Pow :			1,6	
Odour threshold :			No data available	
Vapour density (air = 1) :	(1013 hPa / 20 °C)		1,014	
Oxidising properties :			none	

9.2 Other information

None

SECTION 10: Stability and reactivity

10.1 Reactivity

No information available.

10.2 Chemical stability

No information available.

10.3 Possibility of hazardous reactions

Gases/vapours, flammable

10.4 Conditions to avoid

Take precautionary measures against static discharge. Keep away from sources of ignition. - No smoking.

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10.5 Incompatible materials

Exothermic reaction with: oxidising agent strong acid strong alkali

10.6 Hazardous decomposition products

Decomposition with: Carbon dioxide (CO₂). Carbon monoxide (CO).

SECTION 11: Toxicological information

11.1 Information on toxicological effects

sensitising. May cause an allergic skin reaction.

Acute effects

Acute oral toxicity

Parameter : LD50 (trans-hex-2-enal ; CAS No. : 6728-26-3)
Exposure route : Oral
Species : Rat
Effective dose : 850 mg/kg
Source : Research Institute for Fragrance Materials (RIFM)

Acute dermal toxicity

Parameter : LD50 (trans-hex-2-enal ; CAS No. : 6728-26-3)
Exposure route : Dermal
Species : Rabbit
Effective dose : 600 mg/kg
Source : Research Institute for Fragrance Materials (RIFM)

SECTION 12: Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Based on the n-octanol/water partition coefficient accumulation in organisms is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6 Other adverse effects

Toxic to aquatic life. May cause long lasting harmful effects to aquatic life.

12.7 Further ecological information

None

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Send to a hazardous waste incinerator facility under observation of official regulations. Clean IBCs or drums at approved facility only. Contaminated packages must be completely emptied and can be re-used following proper cleaning. Packing which cannot be properly cleaned must be disposed of. Handle contaminated packages in the same way as the substance itself.

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SECTION 14: Transport information

14.1 UN number

UN 1988

14.2 UN proper shipping name

Land transport (ADR/RID)

ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. (hexenal)

Sea transport (IMDG)

ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. (hexenal)

Air transport (ICAO-TI / IATA-DGR)

ALDEHYDES, FLAMMABLE, TOXIC, N.O.S. (hexenal)

14.3 Transport hazard class(es)

Land transport (ADR/RID)

Class(es) : 3
Classification code : FT1
Hazard identification number (Kemler No.) : 36
Tunnel restriction code : D/E
Special provisions : LQ 5 I · E 1
Hazard label(s) : 3 / 6.1 / N

Sea transport (IMDG)

Class(es) : 3.3
EmS-No. : F-E / S-D
Special provisions : LQ 5 I · E 1 · Segregation Group: No/none
Hazard label(s) : 3 / 6.1 / N

Air transport (ICAO-TI / IATA-DGR)

Class(es) : 3 / 6.1
Special provisions : E 1
Hazard label(s) : 3 / 6.1

14.4 Packing group

III

14.5 Environmental hazards

Land transport (ADR/RID) : Yes

Sea transport (IMDG) : Yes (P)

Air transport (ICAO-TI / IATA-DGR) : Yes

14.6 Special precautions for user

None

SECTION 15: Regulatory information

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

National regulations

Water hazard class (WGK)

Class : water pollutant according VwVwS

Other regulations, restrictions and prohibition regulations

TSCA (USA) : listed

CEPA (Canada) : DSL

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India : not applicable
ENCS (Japan) : listed 2 - 520
ISHL (Japan) : chemical name published
IECSC (China) : listed
ECL (Korea) : listed KE 19843
PICCS (Philippines) : listed
AICS (Australia) : listed
NZIoC (New Zealand) : listed HSR 4976
FLAVIS (EU) : listed 5 - 73
CoE (EU) : listed 748
JECFA (UN) : listed 1353
FEMA (USA) : listed 2560
GRAS (USA) : listed 3

15.2 Chemical Safety Assessment

Chemical safety assessments for substances in this mixture were not carried out.

SECTION 16: Other information

16.1 Indication of changes

02. Classification of the substance or mixture

16.2 Abbreviations and acronyms

a.i. = Active ingredient; ACGIH = American Conference of Governmental Industrial Hygienists (US); ADR = European Agreement concerning the International Carriage of Dangerous Goods by Road; AFFF = Aqueous Film Forming Foam; AICS = Australian Inventory of Chemical Substances; AISE = International Association for Soaps, Detergents and Maintenance Products (joint project of AISE and CEFIC); AOAC = AOAC International (formerly Association of Official Analytical Chemists); aq. = Aqueous; Asia-PAC = Asia Pacific; ASTM = American Society of Testing and Materials (US); atm = Atmosphere(s); B.V. = Beperkt Vennootschap (LTD = Limited); BCF = Bioconcentration Factor; bp = Boiling point at stated pressure; bw = Body weight; ca = (Circa) about; CAS No = Chemical Abstracts Service Number (see ACS - American Chemical Society); CEFIC = European Chemical Industry Council (established 1972); CEPA = Canadian Environmental Protection Act (CAN); CEPA = Canadian Environmental Protection Act (Canada); CIPAC = Collaborative International Pesticides Analytical Council; CLP = REGULATION (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.; CoE = Council of Europe (EU); Conc = Concentration; cP = CentiPoise; CSNN = Chemical Substance Nomination & Notification (Taiwan); cSt = Centistokes; d = Day(s); DIN = Deutsches Institut für Normung e.V.; DNEL = Derived No-Effect Level; DSL = Domestic Substances List; DT50 = Time for 50% loss; half-life; EbC50 = Median effective concentration (biomass, e.g. of algae); EC = European Community; European Commission; EC50 = Median effective concentration; ECL = Existing Chemicals List (Korea); EINECS = European Inventory of Existing Commercial Chemical Substances (EU, outdated, now replaced by EC Number); ELINCS = European List of Notified (New) Chemicals; ENCS = Existing and New Chemical Substances Inventory (Japan); ErC50 = Median effective concentration (growth rate, e.g. of algae); EU = European Union; EWC = European Waste Catalogue; FAO = Food and Agriculture Organization (United Nations); FEMA = Flavor & Extract Manufacturers Association (USA); FLAVIS = Flavour Information System (EU); GIFAP = Groupement International des Associations Nationales de Fabricants de Produits Agrochimiques (now CropLife International); GRAS = Generally Recognized As Safe (USA); h = Hour(s); hPa = HectoPascal (unit of pressure); IARC = International Agency for Research on Cancer; IATA = International Air Transport Association; IC50 = Concentration that produces 50% inhibition; IECSC = Inventory of Existing Chemical Substances (China); IMDG Code = International Maritime Dangerous Goods Code; IMO = International Maritime Organization; ISO = International Organization for Standardization; IUCLID = International Uniform Chemical Information Database; IUPAC = International Union of Pure and Applied Chemistry; IVIS = In-Vitro Irritancy Score; JECFA = Joint Expert Committee on Food Additives (United Nations); kg = Kilogram; Kow = Distribution coefficient between n-octanol and water; kPa = KiloPascal (unit of pressure); LC50 = Concentration required to kill 50% of test organisms; LD50 = Dose required to kill 50% of test organisms; LEL = Lower Explosive Limit/Lower Explosion Limit; LOAEL = Lowest observed adverse effect level; LVE = Low Volume Exemption; mg = Milligram; min = Minute(s); ml = Milliliter; mmHg = Pressure equivalent to 1 mm of mercury (133.3 Pa); mp = Melting point; MRL = Maximum Residue Limit; MSDS = Material Safety Data Sheet; n.o.s. = Not Otherwise Specified; NDSL = Non-Domestic Substances List; NIOSH = National

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Institute for Occupational Safety and Health (US); NOAEL = No Observed Adverse Effect Level; NOEC = No observed effect concentration; NOEL = No Observable Effect Level; NOx = Oxides of Nitrogen; NZIoC = New Zealand Inventory of Chemicals; OECD = Organization for Economic Cooperation and Development; OEL = Occupational Exposure Limits; Pa = Pascal (unit of pressure); PBT = Persistent, Bioaccumulative or Toxic; pH = $-\log_{10}$ hydrogen ion concentration; PICCS = Philippine Inventory of Chemicals and Chemical Substances; pKa = $-\log_{10}$ acid dissociation constant; PNEC = Predicted No Effect Concentration; POPs = Persistent Organic Pollutants; ppb = Parts per billion; PPE = Personal Protection Equipment; ppm = Parts per million; ppt = Parts per trillion; PVC = Polyvinyl Chloride; QSAR = Quantitative Structure-Activity Relationship; REACH = Registration, Evaluation and Authorization of Chemicals (EU, see NCP); SI = International System of Units; STEL = Short-Term Exposure Limit; tech. = Technical grade; TSCA = Toxic Substances Control Act (US); TSCA = Toxic Substances Control Act (USA); TWA = Time-Weighted Average; UN = United Nations; vPvB = Very Persistent and Very Bioaccumulative; VwVwS = Verwaltungsvorschrift wassergefährdender Stoffe; WHO = World Health Organization = OMS; γ = Year(s);

16.3 Key literature references and sources for data

None

16.4 Relevant R-, H- and EUH-phrases (Number and full text)

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H317	May cause an allergic skin reaction.
H411	Toxic to aquatic life with long lasting effects.
10	Flammable.
21/22	Harmful in contact with skin and if swallowed.
43	May cause sensitization by skin contact.
51/53	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

16.5 Training advice

None

16.6 Additional information

None

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.