

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



Trade name : TRANS-2-HEXENYL ACETATE
Revision date : 09.07.2014
Print date : 27-05-2015

Version (Revision) : 2.1.3 (2.1.2)

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

1.1 Product identifier

TRANS-2-HEXENYL ACETATE (W01057)
trans-2-hexenyl acetate ; CAS No. : 2497-18-9 ; EC No. : 219-680-7

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]

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

Hazard classes and hazard categories

Flam. Liq. 3

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

None

2.2 Label elements

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

Hazard pictograms



Flame (GHS02)

Signal word

Warning

Hazard statements

H226 Flammable liquid and vapour.

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Precautionary statements

- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
- P233 Keep container tightly closed.
- P280 Wear protective gloves/protective clothing/eye protection/face protection.
- P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
- P403+P235 Store in a well-ventilated place. Keep cool.
- 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-2-hexenyl acetate

EC No. : 219-680-7

CAS No. : 2497-18-9

Purity : ≥ 97 % [mass]

Synonyms

IUPAC : hex-2-en-1-yl acetate

INCI : TRANS-2-HEXENYL ACETATE

SECTION 4: First aid measures

4.1 Description of first aid measures

General information

When in doubt or if symptoms are observed, get medical advice. 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 respiration.

In case of skin contact

Wash immediately with: Water Do not wash with: Solvents/Thinner

After eye contact

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

Rinse mouth immediately and drink plenty of water. Let water be drunken in little sips (dilution effect). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

No information available.

4.3 Indication of any immediate medical attention and special treatment needed

None

SECTION 5: Firefighting measures

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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.

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. See protective measures under point 7 and 8.

6.2 Environmental precautions

In case of entry into waterways, soil or drains, inform the responsible authorities.

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

7.1 Precautions for safe handling

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work. Wear personal protection equipment (see chapter 8). All work processes must always be designed so that the following is as low as possible: inhalation of vapours or spray/mists. 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.

Hints on joint storage

Keep away from oxidising agent , acid and alkali .

Storage class : 10

Storage class (TRGS 510) : 3

7.3 Specific end use(s)

None

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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

Hand protection is not required

Suitable material : Butyl caoutchouc (butyl rubber)

Breakthrough time (maximum wearing time) : >120 min.

Thickness of the glove material : 1.00 mm.

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 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

Safety relevant basis data

Physical state :		liquid	
Colour :		colourless to pale yellow	
Odour :		sweet, fruity	
Boiling temperature/boiling range : (1013 hPa)		176	°C
Freezing point :	<	-20	°C
Flash point (Closed Cup) :		58	°C
Auto-ignition temperature :			DIN EN 51578
Decomposition temperature		no data available	
Lower explosion limit :		No data available	
Upper explosion limit :		No data available	
Vapour pressure : (20 °C)		0,93	hPa
Relative density (water = 1) : (20 °C)		0,891 - 0,898	
Density : (20 °C)		0,893 - 0,9	g/cm ³
pH value :		No data available	

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Log Pow : 2,6
Viscosity : (20 °C) No data available
Vapour density (air = 1) : (1013 hPa / 20 °C) ca. 1
Oxidising properties : none
Explosive properties : No data available.

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.

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

Acute effects

Acute oral toxicity

Parameter : LD50 (trans-2-hexenyl acetate ; CAS No. : 2497-18-9)
Exposure route : Oral
Species : Rat
Effective dose : > 5 g/kg
Source : Research Institute for Fragrance Materials (RIFM)

Acute dermal toxicity

Parameter : LD50 (trans-2-hexenyl acetate ; CAS No. : 2497-18-9)
Exposure route : Dermal
Species : Rabbit
Effective dose : > 5 g/kg
Source : Research Institute for Fragrance Materials (RIFM)

Irritant and corrosive effects

Primary irritation to the skin

Parameter : Irritation of the skin (trans-2-hexenyl acetate ; CAS No. : 2497-18-9)
Parameter : Rabbit
Exposure time : 24 h
Result : Moderately irritating
Methode : Full strength to intact or abraded skin under occlusion
Source : Research Institute for Fragrance Materials (RIFM)
Parameter : Irritation of the skin (trans-2-hexenyl acetate ; CAS No. : 2497-18-9)

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Parameter : human
Exposure time : 48 h
Result : No irritation
Methode : 10% in petrolatum
Source : Research Institute for Fragrance Materials (RIFM)

SECTION 12: Ecological information

12.1 Toxicity

Aquatic 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

None

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.

SECTION 14: Transport information

14.1 UN number

UN 3272

14.2 UN proper shipping name

Land transport (ADR/RID)

ESTERS, N.O.S. (hexenyl acetate)

Sea transport (IMDG)

ESTERS, N.O.S. (hexenyl acetate)

Air transport (ICAO-TI / IATA-DGR)

ESTERS, N.O.S. (hexenyl acetate)

14.3 Transport hazard class(es)

Land transport (ADR/RID)

Class(es) : 3
Classification code : F1

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Hazard identification number (Kemler No.) : 30
Tunnel restriction code : D/E
Special provisions : LQ 5 I · E 1
Hazard label(s) : 3

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

Air transport (ICAO-TI / IATA-DGR)
Class(es) : 3
Special provisions : E 1
Hazard label(s) : 3

14.4 Packing group

III

14.5 Environmental hazards

Land transport (ADR/RID) : No
Sea transport (IMDG) : No
Air transport (ICAO-TI / IATA-DGR) : No

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
India : not applicable
ENCS (Japan) : listed 2 - 2533
ISHL (Japan) : chemical name published
IECSC (China) : listed
CSNN (Taiwan) : listed
ECL (Korea) : listed KE 19878
PICCS (Philippines) : listed
AICS (Australia) : listed
NZIoC (New Zealand) : group standard
FLAVIS (EU) : listed 9 - 394
CoE (EU) : listed 643
JECFA (UN) : listed 1355
FEMA (USA) : listed 2564
GRAS (USA) : listed 3

15.2 Chemical Safety Assessment

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

SECTION 16: Other information

16.1 Indication of changes

None

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 CroLife 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 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 = -log₁₀ hydrogen ion concentration; PICCS = Philippine Inventory of Chemicals and Chemical Substances; pKa = -log₁₀ 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; y = Year(s);

16.3 Key literature references and sources for data

None

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

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H226 Flammable liquid and vapour.

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.
