

Safety data sheet

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



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

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

date of compilation: 2021-05-19
Revision: 2024-03-02

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

1.1 Product identifier

Identification of the substance	trans-Hexen-2-al ≥98,5 %, for synthesis
Article number	3757
EC number	229-778-1
CAS number	6728-26-3

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

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 sheet: Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	3	Flam. Liq. 3	H226
3.1O	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

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

Precautionary statements

Precautionary statements - prevention

P280 Wear protective gloves/eye protection

Precautionary statements - response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P312 Call a POISON CENTRE/doctor if you feel unwell

2.3 Other hazards

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 $\geq 0,1\%$.

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SECTION 3: Composition/information on ingredients

3.1 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
EC No	229-778-1

Substance, Specific Conc. Limits, M-factors, ATE

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	685 mg/kg 600 mg/kg	oral dermal

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

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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

5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air 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.

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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.

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.

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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 effective 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.

• 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 ° 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)

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Auto-ignition temperature	218 °C at 102 kPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined

Solubility(ies)

Water solubility 5,261 g/l at 25 °C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 1,58 (25 °C) (ECHA)

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

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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.

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

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• **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 $\geq 0,1\%$.

11.3 Information on other hazards

There is no additional information.

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: $2,608 \text{ mg/mg}$
Theoretical Carbon Dioxide: $2,691 \text{ mg/mg}$

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,58 (25 °C) (ECHA)
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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.

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Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

Properties of waste which render it hazardous

HP 3 flammable
HP 6 acute toxicity
HP 13 sensitising

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.

SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 1988
IMDG-Code	UN 1988
ICAO-TI	UN 1988

14.2 UN proper shipping name

ADRRID	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)

ADRRID	3 (6.1)
IMDG-Code	3 (6.1)
ICAO-TI	3 (6.1)

14.4 Packing group

ADRRID	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

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14.8 Information for each of the UN Model Regulations

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) Additional information

Proper shipping name	ALDEHYDES, FLAMMABLE, TOXIC, N.O.S.
Particulars in the transport document	UN1988, ALDEHYDES, FLAMMABLE, TOXIC, N.O.S., (trans-Hexen-2-al), 3 (6.1), III, (D/E)
Classification code	FT1
Danger label(s)	3+6.1
Special provisions (SP)	274, 802(ADN)
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
Transport category (TC)	3
Tunnel restriction code (TRC)	D/E
Hazard identification No	36
Emergency Action Code	3W

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information

Classification code	FT1
Danger label(s)	3+6.1
Special provisions (SP)	274, 802(ADN)
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
Transport category (TC)	3
Hazard identification No	36

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

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Limited quantities (LQ)	5 L
EmS	F-E, S-D
Stowage category	A

International Civil Aviation Organization (ICAO-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

Relevant provisions of the European Union (EU)

Seveso Directive

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
P5c	flammable liquids (cat. 2, 3)	5.000 50.000	51)

Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

Deco-Paint Directive

VOC content	100 %
VOC content	849 g/l

Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	849 g/l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

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Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
trans-Hexen-2-al	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
trans-Hexen-2-al	flammable / pyrophoric		40

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.

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

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Country	Inventory	Status
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

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-relevant
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Danger		yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8		Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information	yes
14.8		Classification code: FT1	yes
14.8		Danger label(s): 3+6.1	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Special provisions (SP): 274, 802(ADN)	yes
14.8		Excepted quantities (EQ): E1	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
14.8		Limited quantities (LQ): 5 L	yes
14.8		Transport category (TC): 3	yes
14.8		Hazard identification No: 36	yes
15.1	Restrictions according to REACH, Annex XVII		yes
15.1		Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table)	yes
15.1	List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed.		yes
15.1	VOC content: 100 % 849 g/l	VOC content: 100 %	yes
15.1		VOC content: 849 g/l	yes
15.1		National regulations(GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed	yes
15.1		Restrictions according to GB REACH, Annex 17	yes
15.1		Dangerous substances with restrictions (GB REACH, Annex 17): change in the listing (table)	yes
15.1		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.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances

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Abbr.	Descriptions of used abbreviations
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
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
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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.