

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



Diacetone alcohol $\geq 98\%$, for synthesis

article number: **3546**

Version: **GHS 4.0 en**

Replaces version of: 2023-04-20

Version: (GHS 3)

date of compilation: 2019-07-01

Revision: 2024-03-02

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

1.1 Product identifier

Identification of the substance	Diacetone alcohol $\geq 98\%$, for synthesis
Article number	3546
CAS number	123-42-2
Alternative name(s)	4-Hydroxy-4-methylpentan-2-one

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
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, 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
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319
3.7	Reproductive toxicity	2	Repr. 2	H361fd

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.8R	Specific target organ toxicity - single exposure (respiratory tract irritation)	3	STOT SE 3	H335

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

Warning

Pictograms

GHS02, GHS07,
GHS08



Hazard statements

H226	Flammable liquid and vapour
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child (if swallowed)

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

Precautionary statements - response

P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
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+P233	Store in a well-ventilated place. Keep container tightly closed
P403+P235	Store in a well-ventilated place. Keep cool

Precautionary statements - disposal

P501	Dispose of contents/container to industrial combustion plant
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For professional users only

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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 $\geq 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Diacetone alcohol
Molecular formula	$C_6H_{12}O_2$
Molar mass	116 g/mol
CAS No	123-42-2

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Irritation, Cough, Dyspnoea

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, 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. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. 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.

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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. Avoid exposure.

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

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. 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:

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)

Cou ntr y	Name of agent	CAS No	Identi- fier	TW A [pp m]	TWA [mg/ m ³]	STE L [pp m]	STEL [mg/ m ³]	Ceil ing- C [pp m]	Ceil- ing-C [mg/ m ³]	Nota- tion	Source
AU	diacetone alcohol (4-hydroxy-4-methylpentan-2-one)	123-42-2	WES	50	238						WES

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

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Notation

STEL	Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)
TWA	Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	32.6 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	240 mg/m ³	human, inhalatory	worker (industry)	acute - local effects
DNEL	467 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	2 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.2 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	100 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	7.4 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.74 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.3 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



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• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. 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

Butyl caoutchouc (butyl rubber)

• material thickness

0,7mm

• 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	clear - light yellow
Odour	faintly perceptible - mild sweet
Melting point/freezing point	-44 °C
Boiling point or initial boiling point and boiling range	166 °C
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	62 g/m ³ (LEL) - 339 g/m ³ (UEL) / 1.2 vol% (LEL) - 6.9 vol% (UEL)
Flash point	58.5 °C at 101.3 kPa (ECHA)
Auto-ignition temperature	515 °C
Decomposition temperature	not relevant
pH (value)	not determined

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Kinematic viscosity	3.426 mm ² /s at 20 °C
Dynamic viscosity	3.22 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	not determined
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	-0.09 (ECHA)
Soil organic carbon/water (log KOC)	0 (ECHA)
Vapour pressure	1.32 hPa at 20 °C
<u>Density and/or relative density</u>	
Density	0.93 – 0.94 g/cm ³ at 20 °C
Relative vapour density	4.01 (air = 1)
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none
9.2 Other information	
Information with regard to physical hazard classes:	There is no additional information.
Other safety characteristics:	
Refractive index	1.422 – 1.425 (20 °C)

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, Bases, Acids, Alkali metals, Amines

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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Rubber articles, different plastics

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

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	3,002 mg/kg	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Suspected of damaging the unborn child (if swallowed). Suspected of damaging fertility (if swallowed).

Specific target organ toxicity - single exposure

May cause respiratory irritation.

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

gastrointestinal complaints, vomiting, nausea

• If in eyes

conjunctivitis (pink eye), Causes serious eye irritation

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- **If inhaled**

Irritation to respiratory tract, cough, Dyspnoea

- **If on skin**

Frequently or prolonged contact with skin may cause dermal irritation

- **Other information**

none

11.2 Endocrine disrupting properties

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

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	$>100 \text{ mg/l}$	fish	ECHA	96 h
EC50	$>1,000 \text{ mg/l}$	aquatic invertebrates	ECHA	48 h
ErC50	$>1,000 \text{ mg/l}$	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
LC50	$>100 \text{ mg/l}$	aquatic invertebrates	ECHA	14 d
EC50	$>100 \text{ mg/l}$	aquatic invertebrates	ECHA	14 d

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.207 mg/mg
Theoretical Carbon Dioxide: 2.276 mg/mg

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
DOC removal	30.54 %	4 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	-0.09 (ECHA)
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12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	0 (ECHA)
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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
H11 Toxic (Delayed or chronic)

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

UN RTDG	UN 1148
IMDG-Code	UN 1148
ICAO-TI	UN 1148

14.2 UN proper shipping name

UN RTDG	DIACETONE ALCOHOL
IMDG-Code	DIACETONE ALCOHOL
ICAO-TI	Diacetone alcohol

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14.3 Transport hazard class(es)

UN RTDG	3
IMDG-Code	3
ICAO-TI	3

14.4 Packing group

UN RTDG	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

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport informationNational regulationsAdditional information(UN RTDG)

UN number	1148
Class	3
Packing group	III
Danger label(s)	3



Special provisions (SP)	223 UN RTDG
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Excepted quantities (EQ)	E1 UN RTDG
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Limited quantities (LQ)	5 L UN RTDG
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Emergency Action Code	2Y
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International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	DIACETONE ALCOHOL
Particulars in the shipper's declaration	UN1148, DIACETONE ALCOHOL, 3, III, 58.5°C c.c.
Marine pollutant	-
Danger label(s)	3



Special provisions (SP)	223
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	Diacetone alcohol
Particulars in the shipper's declaration	UN1148, Diacetone alcohol, 3, III
Danger label(s)	3



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.

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
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	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
CICR	Chemical Inventory and Control Regulation
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
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
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
2.3	Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of ≥ 0,1%.	Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations

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Abbr.	Descriptions of used abbreviations
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
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	Parts per million
STEL	Short-term exposure limit
TWA	Time-weighted average
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne contaminants

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.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child (if swallowed).

Disclaimer

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