

# safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



## Benzoic acid benzyl ester $\geq$ 99% for synthesis

article number: **9498**  
Version: **2.0 en**  
Replaces version of: 2015-07-15  
Version: (1.0)

date of compilation: 2015-07-15  
Revision: 2017-01-26

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

### 1.1 Product identifier

Identification of the substance	<b>Benzoic acid benzyl ester</b>
Article number	9498
Registration number (REACH)	01-2119976371-33-xxxx
Index No	607-085-00-9
EC number	204-402-9
CAS number	120-51-4

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

**Identified uses:** laboratory chemical

### 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](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

**e-mail (competent person)** : [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.10	acute toxicity (oral)	(Acute Tox. 4)	H302
4.1A	hazardous to the aquatic environment - acute hazard	(Aquatic Acute 1)	H400
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 2)	H411

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### Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

## 2.2 Label elements

### Labelling according to Regulation (EC) No 1272/2008 (CLP)

#### Signal word

Warning

#### Pictograms



#### Hazard statements

H302

Harmful if swallowed.

H410

Very toxic to aquatic life with long lasting effects.

#### Precautionary statements

##### Precautionary statements - prevention

P273

Avoid release to the environment.

##### Precautionary statements - response

P301+P312

IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

P330

Rinse mouth.

#### Labelling of packages where the contents do not exceed 125 ml

Signal word: Warning

Symbol(s)



## 2.3 Other hazards

There is no additional information.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Benzoic acid benzyl ester
Index No	607-085-00-9
Registration number (REACH)	01-2119976371-33-xxxx
EC number	204-402-9
CAS number	120-51-4
Molecular formula	C <sub>14</sub> H <sub>12</sub> O <sub>2</sub>
Molar mass	213,3 g/mol

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### 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. In all cases of doubt, or when symptoms persist, seek medical advice.

##### 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

After ingestion: Nausea, Vomiting, Gastrointestinal complaints,

Following inhalation: Cough

#### 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 fire-fighting measures to the fire surroundings  
water spray, foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

water jet

#### 5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

##### Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>)

#### 5.3 Advice for firefighters

Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

##### Special protective equipment for firefighters

Protective clothing against liquid and gaseous chemicals, including liquid aerosols and solid particles. Self-contained breathing apparatus (SCBA). Self-contained breathing apparatus (EN 133). Type: ABEK (combined filters against gases and vapours, colour code: Brown/Grey/Yellow/Green). Type: ABEK-P2 (combined filters against gases, vapours and particles, colour code: Brown/Grey/Yellow/Green/White).

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### SECTION 6: Accidental release measures

#### 6.1 Personal precautions, protective equipment and emergency procedures

##### For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Do not breathe dust. Avoid contact with skin, eyes and clothes.

#### 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

##### Advices on how to contain a spill

Covering of drains.

##### Advices on how to clean up a spill

Take up mechanically. Control of dust.

##### 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.

##### Advice on general occupational hygiene

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

#### 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

##### Incompatible substances or mixtures

Observe hints for combined storage.

##### Consideration of other advice

###### • 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.

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### SECTION 8: Exposure controls/personal protection

#### 8.1 Control parameters

##### National limit values

##### Occupational exposure limit values (Workplace Exposure Limits)

Data are not available.

##### Relevant DNELs/DMELs/PNECs and other threshold levels

###### • human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	102 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	2,6 mg/kg	human, dermal	worker (industry)	chronic - systemic effects
DNEL	5,1 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects

###### • environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0,0168 mg/l	freshwater	short-term (single instance)
PNEC	0,00168 mg/l	marine water	short-term (single instance)
PNEC	100 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	10,66 mg/kg	freshwater sediment	short-term (single instance)
PNEC	1,07 mg/kg	marine sediment	short-term (single instance)
PNEC	2,12 mg/kg	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

###### • 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.

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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

Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

Respiratory protection necessary at: Dust formation.

Observe the wear time limits according GefStoffV in combination with the rules for using respiratory protection apparatus (BGR 190).

### 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

#### Appearance

Physical state	solid (solid matter)
Colour	colourless
Odour	this information is not available
Odour threshold	No data available

#### Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	21 °C
Initial boiling point and boiling range	323,5 °C
Flash point	148 °C at 101,3 kPa
Evaporation rate	no data available
Flammability (solid, gas)	Non-flammable
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	<0,1 hPa at 20 °C
Density	1,12 g/cm <sup>3</sup>
Vapour density	7,31 (air = 1)
Relative density	Information on this property is not available.

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### Solubility(ies)

Water solubility no data available

### Partition coefficient

n-octanol/water (log KOW) 3,97 (25 °C) (ECHA)

Soil organic carbon/water (log KOC) 3,8 (40 °C) (ECHA)

Auto-ignition temperature 480 °C - ECHA

Decomposition temperature no data available

Viscosity not relevant (solid matter)

• dynamic viscosity 10,9 mPa s at 25 °C

Explosive properties Shall not be classified as explosive

Oxidising properties none

## 9.2 Other information

Temperature class (EU, acc. to ATEX) T1 (Maximum permissible surface temperature on the equipment: 450°C)

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

### 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

Exothermic reaction with: Alkali metals, Aluminium, Strong oxidiser

### 10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

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### SECTION 11: Toxicological information

#### 11.1 Information on toxicological effects

##### Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	1.900 mg/kg	rat	ECHA

##### 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

Shall not be classified as a respiratory or skin sensitiser.

##### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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

nausea, vomiting, gastrointestinal complaints

##### • If in eyes

data are not available

##### • If inhaled

data are not available

##### • If on skin

data are not available

##### Other information

None



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### SECTION 12: Ecological information

#### 12.1 Toxicity

Toxic to aquatic life with long lasting effects.

##### Aquatic toxicity (acute)

Very toxic to aquatic organisms.

Endpoint	Value	Species	Source	Exposure time
LC50	2,32 mg/l	fish	ECHA	96 h
EC50	3,09 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	0,475 mg/l	algae	ECHA	72 h

##### Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

Endpoint	Value	Species	Source	Exposure time
EC50	4,26 mg/l	aquatic invertebrates	ECHA	24 h
LC50	11 mg/l	aquatic invertebrates	ECHA	24 h
NOEC	0,258 mg/l	aquatic invertebrates	ECHA	21 d
LOEC	0,455 mg/l	aquatic invertebrates	ECHA	21 d

#### 12.2 Process of degradability

The substance is readily biodegradable.  
Theoretical Oxygen Demand: 2,401 mg/mg  
Theoretical Carbon Dioxide: 2,889 mg/mg

Process	Degradation rate	Time
biotic/abiotic	94 %	28 d
oxygen depletion	94 %	28 d

#### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) 3,97 (25 °C)

#### 12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient 3,8 (40 °C)

#### 12.5 Results of PBT and vPvB assessment

Data are not available.

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### 12.6 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. Avoid release to the environment. Refer to special instructions/safety data sheets.

#### Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

### 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.

### 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.

## SECTION 14: Transport information

14.1	UN number	3077
14.2	UN proper shipping name	<b>ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.</b>
	Hazardous ingredients	Benzoic acid benzyl ester
14.3	Transport hazard class(es)	
	Class	9 (miscellaneous dangerous substances and articles) (environmentally hazardous)
14.4	Packing group	III (substance presenting low danger)
14.5	Environmental hazards	hazardous to the aquatic environment
14.6	<b>Special precautions for user</b>	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7	<b>Transport in bulk according to Annex II of MARPOL and the IBC Code</b>	
	The cargo is not intended to be carried in bulk.	
14.8	<b>Information for each of the UN Model Regulations</b>	
	<b>• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)</b>	
	UN number	3077
	Proper shipping name	<b>ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.</b>
	Particulars in the transport document	UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzoic acid benzyl ester), 9, III, (-)
	Class	9
	Classification code	M7
	Packing group	III

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Danger label(s)	9 + "fish and tree"
Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	274, 335, 375, 601
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	3
Tunnel restriction code (TRC)	-
Hazard identification No	90
<b>Emergency Action Code</b>	2Z
<b>• International Maritime Dangerous Goods Code (IMDG)</b>	
UN number	3077
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
Particulars in the shipper's declaration	UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzoic acid benzyl ester), 9, III
Class	9
Marine pollutant	yes (hazardous to the aquatic environment)
Packing group	III
Danger label(s)	9 + "fish and tree"
Special provisions (SP)	274, 335, 966, 967, 969
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
EmS	F-A, S-F
Stowage category	A
<b>• International Civil Aviation Organization (ICAO-IATA/DGR)</b>	
UN number	3077
Proper shipping name	Environmentally hazardous substance, solid, n.o.s.
Particulars in the shipper's declaration	UN3077, Environmentally hazardous substance, solid, n.o.s., (Benzoic acid benzyl ester), 9, III
Class	9
Environmental hazards	yes (hazardous to the aquatic environment)

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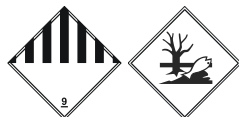
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Packing group

III

9 + "fish and tree"



Special provisions (SP)

A97, A158, A179, A197, 274

Excepted quantities (EQ)

E1

Limited quantities (LQ)

30 kg

## 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)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**  
Not listed.
- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**  
Not listed.
- **Regulation 850/2004/EC on persistent organic pollutants (POP)**  
Not listed.
- **List of substances subject to authorisation (REACH, Annex XIV)**  
not listed
- **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
E1	environmental hazards (hazardous to the aquatic environment, cat. 1)	100                      200	56)

#### Notation

56) Hazardous to the Aquatic Environment in category Acute 1 or Chronic 1

#### Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

#### Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

#### Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

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### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

### 15.2 Chemical Safety Assessment

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

## SECTION 16: Other information

### 16.1 Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)
2.2		Pictograms: change in the listing (table)
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)
8.1		• environmental values: change in the listing (table)
14.2	Hazardous ingredients: Benzyl benzoate	Hazardous ingredients: Benzoic acid benzyl ester
14.8	Particulars in the transport document: UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzyl benzoate), 9, III, (E)	Particulars in the transport document: UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzoic acid benzyl ester), 9, III, (-)
14.8	Tunnel restriction code (TRC): E	Tunnel restriction code (TRC): -
14.8		Emergency Action Code: 2Z
14.8	Particulars in the shipper's declaration: UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzyl benzoate), 9, III	Particulars in the shipper's declaration: UN3077, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S., (Benzoic acid benzyl ester), 9, III
14.8		• International Civil Aviation Organization (ICAO-IATA/DGR)
14.8		UN number: 3077
14.8		Proper shipping name: Environmentally hazardous substance, solid, n.o.s.
14.8		Particulars in the shipper's declaration: UN3077, Environmentally hazardous substance, solid, n.o.s., (Benzoic acid benzyl ester), 9, III
14.8		Class: 9
14.8		Environmental hazards: yes (hazardous to the aquatic environment)
14.8		Packing group: III9 + "fish and tree"
14.8		Packing group: change in the listing (table)
14.8		Special provisions (SP): A97, A158, A179, A197, 274
14.8		Excepted quantities (EQ): E1

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Section	Former entry (text/value)	Actual entry (text/value)
14.8		Limited quantities (LQ): 30 kg

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
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 Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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)
vPvB	very Persistent and very Bioaccumulative

### Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

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

Code	Text
H302	harmful if swallowed
H400	very toxic to aquatic life
H411	toxic to aquatic life with long lasting effects

### Disclaimer

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.