

Safety Data Sheet

according to Regulation (EC) No 1907/2006

4-tert-Butylcatechol > 98.0 %

Revision date: 24.11.2022

Product code: 25428

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

1.1. Product identifier

4-tert-Butylcatechol > 98.0 %

Substance name: 4-tert-butylpyrocatechol
CAS No: 98-29-3
EC No: 202-653-9

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

Use of the substance/mixture

Laboratory chemicals

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: Fa. Bernd Kraft GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
e-mail: info@berndkraft.de
Contact person: Abteilung Produktsicherheit
e-mail: produktsicherheit@berndkraft.de
Internet: www.berndkraft.de
Responsible Department: Abteilung Produktsicherheit

Telefax: 0203/5194-290

Telephone: 0203/5194-107/117

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Carc. 1B; H350
Acute Tox. 4; H312
Acute Tox. 4; H302
Skin Corr. 1B; H314
Eye Dam. 1; H318
Skin Sens. 1; H317
Aquatic Acute 1; H400
Aquatic Chronic 2; H411

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

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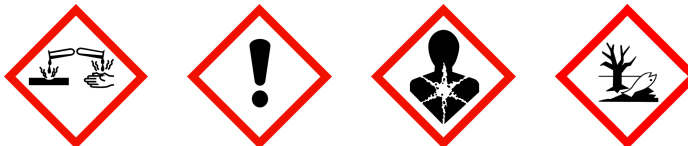
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Pictograms:



Hazard statements

- H302+H312 Harmful if swallowed or in contact with skin.
- H314 Causes severe skin burns and eye damage.
- H317 May cause an allergic skin reaction.
- H350 May cause cancer.
- H400 Very toxic to aquatic life.
- H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

- P260 Do not breathe dust/fume/gas/mist/vapours/spray.
- 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 or shower.
- P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P310 Immediately call a POISON CENTER/doctor.

Special labelling of certain mixtures

Restricted to professional users.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₁₀H₁₄O₂
Molecular weight: 166,22 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	Classification (Regulation (EC) No 1272/2008)	
98-29-3	4-tert-butylpyrocatechol	100 %
	202-653-9	
	Carc. 1B, Acute Tox. 4, Acute Tox. 4, Skin Corr. 1B, Eye Dam. 1, Skin Sens. 1, Aquatic Acute 1, Aquatic Chronic 2; H350 H312 H302 H314 H318 H317 H400 H411	
120-80-9	1,2-dihydroxybenzene	< 1 %
	204-427-5	
	604-016-00-4	
	01-2119515921-43-XXXX	
	Carc. 1B, Muta. 2, Acute Tox. 3, Acute Tox. 3, Acute Tox. 4, Skin Irrit. 2, Eye Dam. 1, Skin Sens. 1; H350 H341 H311 H301 H332 H315 H318 H317	

Full text of H and EUH statements: see section 16.

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
98-29-3	202-653-9	4-tert-butylpyrocatechol	100 %
		dermal: LD50 = 1331 mg/kg; oral: LD50 = 815 mg/kg	
120-80-9	204-427-5	1,2-dihydroxybenzene	< 1 %
		inhalation: ATE = 11 mg/l (vapours); inhalation: ATE = 1,5 mg/l (dusts or mists); dermal: ATE 600 mg/kg; oral: ATE 300 mg/kg	

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

Self-protection of the first aider

After inhalation

Provide fresh air.
Call a physician immediately.

After contact with skin

Wash immediately with: Water
In case of skin contact, wash immediately with large quantities of water/polyethylene glycol 400 (Roticlean).
Take off immediately all contaminated clothing and wash it before reuse.
Call a physician immediately.

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.
Remove contact lenses, if present and easy to do. Continue rinsing.

After ingestion

Rinse mouth immediately and drink plenty of water.
Do NOT induce vomiting.
Do not allow a neutralisation agent to be drunk.
Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Irritant
corrosive
Cough
Dyspnoea
Circulatory collapse
Allergic reactions
Risk of serious damage to eyes.
Methaemoglobinaemia

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO2)
Foam

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Extinguishing powder
Water

Unsuitable extinguishing media
no restriction

5.2. Special hazards arising from the substance or mixture

Combustible solids
Hazardous combustion products
In case of fire may be liberated: Carbon dioxide (CO₂) Carbon monoxide
In case of warming: Vapours are heavier than air, spread along floors and form explosive mixtures with air.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.
In case of fire and/or explosion do not breathe fumes.
Avoid contact with skin, eyes and clothes.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Move undamaged containers from immediate hazard area if it can be done safely.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
Emergency procedures
Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.
Prevent spread over a wide area (e.g. by containment or oil barriers).
Collect in closed and suitable containers for disposal.
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.
Do not breathe dust/fume/gas/mist/vapours/spray.
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7
Personal protection equipment: see section 8
Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

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Advice on safe handling

Read label before use. Handle and open container with care.
When using do not eat, drink, smoke, sniff. Keep container tightly closed.
Use personal protection equipment. Use extractor hood (laboratory).
Avoid dust formation. Do not breathe dust.
Provide adequate ventilation.

Advice on protection against fire and explosion

Take action to prevent static discharges. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.
Wash hands and face before breaks and after work and take a shower if necessary.
When using do not eat or drink.
Avoid: aerosol or mist formation Do not breathe vapour/aerosol.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.
Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. If handled uncovered, arrangements with local exhaust ventilation have to be used.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place.
Store in a cool dry place.
Protect against: Light
Store in a place accessible by authorized persons only.

Further information on storage conditions

Protect from sunlight.
storage temperature < 30°C
Store in a place accessible by authorized persons only.

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Occupational exposure limits

CAS No	Substance	ppm	mg/m ³	fib/cm ³	Category	Origin
120-80-9	Pyrocatechol	5	20		TWA (8 h)	

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DNEL/DMEL values

CAS No	Substance		
DNEL type	Exposure route	Effect	Value
98-29-3	4-tert-butylpyrocatechol		
Worker DNEL, long-term	inhalation	systemic	1,6 mg/m ³
Consumer DNEL, long-term	oral	systemic	0,117 mg/kg bw/day
Consumer DNEL, acute	oral	systemic	1,6 mg/kg bw/day
120-80-9	1,2-dihydroxybenzene		
Worker DNEL, long-term	inhalation	systemic	1 mg/m ³
Worker DNEL, acute	inhalation	systemic	85 mg/m ³
Worker DNEL, acute	dermal	systemic	2,5 mg/kg bw/day
Consumer DNEL, long-term	inhalation	systemic	0,3 mg/m ³
Consumer DNEL, acute	inhalation	systemic	63 mg/m ³
Consumer DNEL, acute	dermal	systemic	1 mg/kg bw/day
Consumer DNEL, long-term	oral	systemic	0,1 mg/kg bw/day
Consumer DNEL, acute	oral	systemic	16 mg/kg bw/day

PNEC values

CAS No	Substance	
Environmental compartment	Value	
98-29-3	4-tert-butylpyrocatechol	
Freshwater	0,0012 mg/l	
Freshwater (intermittent releases)	0,0012 mg/l	
Marine water	0,00012 mg/l	
Freshwater sediment	0,0069 mg/kg	
Marine sediment	0,00069 mg/kg	
Micro-organisms in sewage treatment plants (STP)	0,16 mg/l	
Soil	0,00068 mg/kg	
120-80-9	1,2-dihydroxybenzene	
Freshwater	0,0011 mg/l	
Freshwater (intermittent releases)	0,011 mg/l	
Marine water	0,00011 mg/l	
Freshwater sediment	0,017 mg/kg	
Marine sediment	0,002 mg/kg	
Micro-organisms in sewage treatment plants (STP)	1,958 mg/l	
Soil	0,003 mg/kg	

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles

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Face protection umbrella

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. 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.

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation KCL 741 Dermatril® L

Suitable material: NBR (Nitrile rubber) 0,11 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation KCL 741 Dermatril® L

Suitable material: NBR (Nitrile rubber) 0,11 mm

Wearing time with occasional contact (splashes): > 480 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

Protective clothing

Take off immediately all contaminated clothing and wash it before reuse.

Wear suitable protective clothing. Take off immediately all contaminated clothing.

Wash hands and face before breaks and after work and take a shower if necessary.

Respiratory protection

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

Filtering device with filter or ventilator filtering device of type: P2

Environmental exposure controls

Do not allow to enter into surface water or drains.

Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	solid	
Colour:	beige	
Odour:	like: Phenol	
Odour threshold:	No data available	
Melting point/freezing point:		52-55 °C
Boiling point or initial boiling point and boiling range:		290,5 °C
Flammability		
Solid/liquid:		No data available
Gas:		No data available
Lower explosion limits:		No data available
Upper explosion limits:		No data available

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Flash point:	130 °C
Auto-ignition temperature:	160 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic: (at 57 °C)	100 mm ² /s
Water solubility: (at 20 °C)	2 g/L
Solubility in other solvents	No data available
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapour pressure: (at 20 °C)	0,01095 hPa
Vapour pressure: (at 107 °C)	13,3 hPa
Density:	1,05 g/cm ³
Relative density:	No data available
Bulk density:	650-700 kg/m ³
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

In case of warming:

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

Sustaining combustion: Sustaining combustion

Self-ignition temperature

Solid: No data available

Gas: No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate: No data available

Solvent separation test: No data available

Solvent content: No data available

Solid content: 100%

Sublimation point: No data available

Softening point: No data available

Pour point: No data available

: No data available

Viscosity / dynamic: No data available

Flow time: No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Danger of dust explosion.

In case of warming:

Vapours may form explosive mixtures with air.

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10.2. Chemical stability

Protect against:
Light
Humidity

10.3. Possibility of hazardous reactions

Oxidising agent
Alkali (lye)
Strong acid

10.4. Conditions to avoid

Heat
Light
Humidity

10.5. Incompatible materials

No data available

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Harmful if swallowed.
Harmful in contact with skin.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
98-29-3	4-tert-butylpyrocatechol				
	oral	LD50 815 mg/kg	Rat	Study report (1992)	OECD Guideline 401
	dermal	LD50 1331 mg/kg	Rat	Study report (1992)	OECD Guideline 402
120-80-9	1,2-dihydroxybenzene				
	oral	ATE 300 mg/kg			
	dermal	ATE 600 mg/kg			
	inhalation vapour	ATE 11 mg/l			
	inhalation dust/mist	ATE 1,5 mg/l			

Irritation and corrosivity

Causes severe skin burns and eye damage.
Causes serious eye damage.

Sensitising effects

May cause an allergic skin reaction. (4-tert-butylpyrocatechol; 1,2-dihydroxybenzene)

Carcinogenic/mutagenic/toxic effects for reproduction

May cause cancer. (4-tert-butylpyrocatechol; 1,2-dihydroxybenzene)
Germ cell mutagenicity: Based on available data, the classification criteria are not met.
Reproductive toxicity: Based on available data, the classification criteria are not met.

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STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

Further information

Irritant
corrosive
Cough
Dyspnoea
Circulatory collapse
Allergic reactions
Risk of serious damage to eyes.
Methaemoglobinaemia

SECTION 12: Ecological information

12.1. Toxicity

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
98-29-3	4-tert-butylpyrocatechol					
	Acute fish toxicity	LC50 mg/l	0,12	96 h	Danio rerio	Study report (2010) OECD Guideline 203
	Acute algae toxicity	ErC50 mg/l	10,17	72 h	Pseudokirchneriella subcapitata	Study report (2010) OECD Guideline 201
	Crustacea toxicity	NOEC mg/l	0,135	21 d	Daphnia magna	Study report (2013) OECD Guideline 211
	Acute bacteria toxicity	(EC50	16 mg/l)	3 h	activated sludge of a predominantly domestic sewage	Study report (2009) OECD Guideline 209
120-80-9	1,2-dihydroxybenzene					
	Acute fish toxicity	LC50 mg/l	9,22	96 h	Pimephales promelas	Center for Lake Superior Environmental s OECD Guideline 203
	Acute algae toxicity	ErC50	22 mg/l	96 h	Chlorella vulgaris	Polish Journal of Environmental Studies, OECD Guideline 201

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12.2. Persistence and degradability

24,7 %; 28 d

Not readily biodegradable (according to OECD criteria)

12.3. Bioaccumulative potential

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
98-29-3	4-tert-butylpyrocatechol	103,66
120-80-9	1,2-dihydroxybenzene	0,88

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

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

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

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

No data available

12.7. Other adverse effects

Avoid release to the environment.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Send to a physico-chemical treatment facility under observation of official regulations.

Do not empty into drains.

Contaminated packaging

Handle contaminated packages in the same way as the substance itself.

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

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number:	UN 3261
14.2. UN proper shipping name:	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-tert-butylpyrocatechol)
14.3. Transport hazard class(es):	8
14.4. Packing group:	II
Hazard label:	8
Classification code:	C4
Special Provisions:	274
Limited quantity:	1 kg
Excepted quantity:	E2
Transport category:	2
Hazard No:	80
Tunnel restriction code:	E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 3261
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14.2. UN proper shipping name:	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-tert-butylpyrocatechol)
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Hazard label:	8
Classification code:	C4
Special Provisions:	274
Limited quantity:	1 kg
Excepted quantity:	E2

Marine transport (IMDG)

14.1. UN number or ID number:	UN 3261
14.2. UN proper shipping name:	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-tert-butylpyrocatechol)
14.3. Transport hazard class(es):	8
14.4. Packing group:	II
Hazard label:	8
Special Provisions:	274
Limited quantity:	1 kg
Excepted quantity:	E2
EmS:	F-A, S-B
Segregation group:	1 - acids

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 3261
14.2. UN proper shipping name:	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-tert-butylpyrocatechol)
14.3. Transport hazard class(es):	8
14.4. Packing group:	II
Hazard label:	8
Special Provisions:	A3 A803
Limited quantity Passenger:	5 kg
Passenger LQ:	Y844
Excepted quantity:	E2
IATA-packing instructions - Passenger:	859
IATA-max. quantity - Passenger:	15 kg
IATA-packing instructions - Cargo:	863
IATA-max. quantity - Cargo:	50 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS:	Yes
Danger releasing substance:	4-tert-butylpyrocatechol

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 28, Entry 75

Information according to 2012/18/EU (SEVESO III): E1 Hazardous to the Aquatic Environment

National regulatory information

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Employment restrictions:	Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.
Water hazard class (D):	3 - highly hazardous to water

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 1,2,14,15.

Relevant H and EUH statements (number and full text)

H301	Toxic if swallowed.
H302	Harmful if swallowed.
H302+H312	Harmful if swallowed or in contact with skin.
H311	Toxic in contact with skin.
H312	Harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H332	Harmful if inhaled.
H341	Suspected of causing genetic defects if swallowed.
H350	May cause cancer.
H400	Very toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

Further Information

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. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.