

Safety Data Sheet

according to Regulation (EC) No 1907/2006

p-Toluenesulfonyl isocyanate solution 40 ml p-toluenesulfonyl isocyanate/l in acetonitrile for deter

Revision date: 26.11.2024

Product code: 26791

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

1.1. Product identifier

p-Toluenesulfonyl isocyanate solution 40 ml p-toluenesulfonyl isocyanate/l in acetonitrile for deter

UFI: 046D-22KF-200F-S0AN

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

Use of the substance/mixture

Laboratory chemical

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: AnalytiChem GmbH

ACD

Street: Stempelstraße 6

Place: D-47167 Duisburg

Telephone: 0203/5194-0

Telefax: 0203/5194-290

E-mail: info@analytichem.de

Contact person: Abteilung Produktsicherheit

Telephone: 0203/5194-107/117

E-mail: produktsicherheit@analytichem.de

Internet: www.analytichem.de

Responsible Department: Abteilung Produktsicherheit

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

This product is a mixture. REACH Registration Number see section 3.

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 2; H225

Acute Tox. 4; H302

Acute Tox. 4; H312

Acute Tox. 4; H332

Eye Irrit. 2; H319

Resp. Sens. 1; H334

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Hazard components for labelling

acetonitrile

4-isocyanatosulphonyltoluene

Signal word: Danger

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Pictograms:



Hazard statements

- H225 Highly flammable liquid and vapour.
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statements

- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P342+P311 If experiencing respiratory symptoms: Call a POISON CENTER/doctor.
P403+P235 Store in a well-ventilated place. Keep cool.

Special labelling of certain mixtures

- EUH204 Contains isocyanates. May produce an allergic reaction.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
75-05-8	acetonitrile			95 - < 100 %
	200-835-2	608-001-00-3	01-2119471307-38	
	Flam. Liq. 2, Acute Tox. 4, Acute Tox. 4, Acute Tox. 4, Eye Irrit. 2; H225 H332 H312 H302 H319			
4083-64-1	4-isocyanatosulphonyltoluene			1 - < 5 %
	223-810-8	615-012-00-7		
	Acute Tox. 3, Skin Irrit. 2, Eye Irrit. 2, Resp. Sens. 1, STOT SE 3; H331 H315 H319 H334 H335 EUH014			

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

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
75-05-8	200-835-2	acetonitrile	95 - < 100 %
	inhalation: LC50 = 3587 mg/l (vapours); inhalation: ATE = 1,5 mg/l (dusts or mists); dermal: LD50 = > 2000 mg/kg; oral: LD50 = 469 mg/kg		
4083-64-1	223-810-8	4-isocyanatosulphonyltoluene	1 - < 5 %
	inhalation: ATE = 3 mg/l (vapours); inhalation: ATE = 0,5 mg/l (dusts or mists) Skin Irrit. 2; H315: >= 5 - 100 Eye Irrit. 2; H319: >= 5 - 100 STOT SE 3; H335: >= 5 - 100		

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).

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SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.

If breathing is irregular or stopped, administer artificial respiration.

Call a physician immediately.

After contact with skin

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

Call a physician immediately.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

After ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

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

Headache

Dyspnoea

Irritant

Vomiting

Spasms

Unconsciousness

Respiratory complaints

Cardiac arrhythmias

Dizziness

Release of: Hydrogen cyanide (hydrocyanic acid)

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

Water spray jet, Carbon dioxide (CO₂), Foam, Extinguishing powder.

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquid.

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 dioxide (CO₂), Carbon monoxide

Hydrogen cyanide (hydrocyanic acid)

Beware of reignition.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Danger of bursting container.

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Use water spray jet to protect personnel and to cool endangered containers.
Suppress gases/vapours/mists with water spray jet.
Move undamaged containers from immediate hazard area if it can be done safely.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.
This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).
Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
Emergency procedures
Consult an expert
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.
The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.
Danger of explosion

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

Advice on safe handling

Read label before use. Handle and open container with care.
When using do not eat, drink, smoke, sniff. Use personal protection equipment.
Provide adequate ventilation. Avoid contact with skin, eyes and clothes.

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Do not breathe vapour/aerosol. Use extractor hood (laboratory).

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.
Vapours can form explosive mixtures with air.

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

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. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Further information on storage conditions

Keep container dry.
storage temperature: +5°C - +30°C

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
75-05-8	Acetonitrile	40	70		TWA (8 h)	

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
75-05-8	acetonitrile			
Worker DNEL, long-term	inhalation	systemic	68 mg/m ³	
Worker DNEL, acute	inhalation	systemic	68 mg/m ³	
Worker DNEL, long-term	inhalation	local	68 mg/m ³	
Worker DNEL, acute	inhalation	local	68 mg/m ³	
Worker DNEL, long-term	dermal	systemic	32,2 mg/kg bw/day	
Consumer DNEL, long-term	inhalation	systemic	4,8 mg/m ³	
Consumer DNEL, acute	inhalation	systemic	220 mg/m ³	
Consumer DNEL, long-term	inhalation	local	4,8 mg/m ³	
Consumer DNEL, acute	inhalation	local	22 mg/m ³	
Consumer DNEL, acute	oral	systemic	0,6 mg/kg bw/day	

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PNEC values

CAS No	Substance	
Environmental compartment		Value
75-05-8	acetonitrile	
Freshwater		10 mg/l
Freshwater (intermittent releases)		10 mg/l
Marine water		1 mg/l
Freshwater sediment		7,53 mg/kg
Micro-organisms in sewage treatment plants (STP)		32 mg/l
Soil		2,41 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

Suitable eye protection: goggles.

Hand protection

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

Recommended glove articles: KCL 897 Butoject®

Recommended material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Recommended glove articles: KCL 897 Butoject®

Recommended material: Butyl caoutchouc (butyl rubber) 0,3 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

Flame-retardant protective clothing. Wear anti-static footwear and clothing

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not allow to enter into surface water or drains.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

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Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid	
Colour:	colourless	
Odour:	characteristic	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		~81 °C
Flammability:		not applicable
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		~2 °C
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic:		No data available
Water solubility:		No data available
Solubility in other solvents		
not determined		
Partition coefficient n-octanol/water:		No data available
Vapour pressure:		No data available
Vapour pressure:		No data available
Density:		0,792 g/cm³
Bulk density:		No data available
Relative vapour density:		No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

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

Sustaining combustion:

Sustaining combustion

Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

Oxidizing properties

Not oxidising.

Other safety characteristics

Evaporation rate:	No data available
Solvent separation test:	No data available
Solvent content:	No data available
Solid content:	No data available
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

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SECTION 10: Stability and reactivity

10.1. Reactivity

There are no data available on the mixture itself.

10.2. Chemical stability

Keep away from heat.

10.3. Possibility of hazardous reactions

Oxidising agent

10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.

10.5. Incompatible materials

Rubber articles
Plastic articles

10.6. Hazardous decomposition products

In case of fire may be liberated:

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

There are no data available on the mixture itself.

Acute toxicity

Harmful if swallowed.
Harmful in contact with skin.
Harmful if inhaled.

ATEmix calculated

ATE (oral) 478,6 mg/kg; ATE (dermal) 1122 mg/kg; ATE (inhalation vapour) 10,44 mg/l; ATE (inhalation dust/mist) 1,442 mg/l

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
75-05-8	acetonitrile				
	oral	LD50 469 mg/kg	Mouse	Study report (1998)	OECD Guideline 401
	dermal	LD50 > 2000 mg/kg	Rabbit	Study report (1997)	OECD Guideline 402
	inhalation (4 h) vapour	LC50 3587 mg/l	Mouse	Study report (1998)	OECD Guideline 403
	inhalation dust/mist	ATE 1,5 mg/l			
4083-64-1	4-isocyanatosulphonyltoluene				
	inhalation vapour	ATE 3 mg/l			
	inhalation dust/mist	ATE 0,5 mg/l			

Irritation and corrosivity

Serious eye damage/eye irritation: Causes serious eye irritation.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

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Sensitising effects

May cause allergy or asthma symptoms or breathing difficulties if inhaled. (4-isocyanatosulphonyltoluene)
Contains isocyanates. May produce an allergic reaction.

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.
Carcinogenicity: Based on available data, the classification criteria are not met.
Reproductive toxicity: Based on available data, the classification criteria are not met.

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.

Specific effects in experiment on an animal

There are no data available on the mixture itself.

Additional information on tests

There are no data available on the mixture itself.

Practical experience

There are no data available on the mixture itself.

11.2. Information on other hazards

Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to humans as no components meets the criteria.

Other information

Headache
Dyspnoea
Irritant
Vomiting
Spasms
Unconsciousness
Respiratory complaints
Cardiac arrhythmias
Dizziness
Release of: Hydrogen cyanide (hydrocyanic acid)

Further information

There are no data available on the mixture itself.

SECTION 12: Ecological information

12.1. Toxicity

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

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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
75-05-8	acetonitrile					
	Acute fish toxicity	LC50 mg/l	1640	96 h	Pimephales promelas	Review article or handbook (1984)
	Acute algae toxicity	ErC50 mg/l	3560	72 h	Phaeodactylum tricornutum	Study report (2010)
	Acute crustacea toxicity	EC50 mg/l	3600	48 h	Daphnia magna	Bull. Environ. Contam. Toxicol. 57:655-6
	Fish toxicity	NOEC	102 mg/l	7 d	Oryzias latipes	Study report (1996)
	Crustacea toxicity	NOEC	960 mg/l	21 d	Daphnia magna	Study report (1996)

12.2. Persistence and degradability

Readily biodegradable (according to OECD criteria).

12.3. Bioaccumulative potential

There are no data available on the mixture itself.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
75-05-8	acetonitrile	0,29

BCF

CAS No	Chemical name	BCF	Species	Source
75-05-8	acetonitrile	3		HSDB (2009)

12.4. Mobility in soil

There are no data available on the mixture itself.

12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

12.6. Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

12.7. Other adverse effects

There are no data available on the mixture itself.

Further information

There are no data available on the mixture itself.

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.
Do not mix with other wastes.

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.

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SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number:	UN 1648
14.2. UN proper shipping name:	ACETONITRILE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	33
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 1648
14.2. UN proper shipping name:	ACETONITRILE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2

Marine transport (IMDG)

14.1. UN number or ID number:	UN 1648
14.2. UN proper shipping name:	ACETONITRILE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Special Provisions:	-
Limited quantity:	1 L
Excepted quantity:	E2
EmS:	F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 1648
14.2. UN proper shipping name:	ACETONITRILE
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3
Limited quantity Passenger:	1 L
Passenger LQ:	Y341
Excepted quantity:	E2
IATA-packing instructions - Passenger:	353
IATA-max. quantity - Passenger:	5 L
IATA-packing instructions - Cargo:	364
IATA-max. quantity - Cargo:	60 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Combustible liquid.

14.7. Maritime transport in bulk according to IMO instruments

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not applicable

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 40, Entry 75

Information according to Directive
2012/18/EU (SEVESO III):

P5c FLAMMABLE LIQUIDS

National regulatory information

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):

2 - obviously hazardous to water

Skin resorption/Sensitization:

Permeates easily through outer skin and causes poisoning.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 1,9,11.

Abbreviations and acronyms

Flam. Liq: Flammable liquid

Acute Tox: Acute toxicity

Skin Irrit: Skin irritation

Eye Irrit: Eye irritation

Resp. Sens: Respiratory sensitisation

STOT SE: Specific target organ toxicity - single exposure

ADR: Accord européen sur le transport des marchandises dangereuses par Route

(European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

Classification for mixtures and used evaluation method according to Regulation (EC) No 1272/2008 [CLP]

Classification	Classification procedure
Flam. Liq. 2; H225	On basis of test data
Acute Tox. 4; H302	Calculation method
Acute Tox. 4; H312	Calculation method
Acute Tox. 4; H332	Calculation method
Eye Irrit. 2; H319	Calculation method
Resp. Sens. 1; H334	Calculation method

Relevant H and EUH statements (number and full text)

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H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H302+H312+H332	Harmful if swallowed, in contact with skin or if inhaled.
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H332	Harmful if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.
EUH014	Reacts violently with water.
EUH204	Contains isocyanates. May produce an allergic reaction.

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. Provide appropriate information, instructions and training to users

(The data for the relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)