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

1.1 Product identifier	
Trade name :	thermosept® SKS
1.2 Relevant identified uses of the	substance or mixture and uses advised against
Use of the Sub- : stance/Mixture	Decalcification agent
Recommended restrictions : on use	Restricted to professional users.
1.3 Details of the supplier of the sa	afety data sheet
Producer :	Schülke & Mayr GmbH Robert-Koch-Str. 2
	22851 Norderstedt Germany Telephone: +49 (0)40/ 52100-0 Telefax: +49 (0)40/ 52100318 mail@schuelke.com www.schuelke.com
Supplier :	Schülke & Mayr UK Ltd. Cygnet House 1, Jenkin Road
	Sheffield S9 1AT United Kingdom Telephone: +44 114 254 35 00 Telefax: +44 114 254 35 01 mail.uk@schulke.com
E-mail address of person : responsible for the SDS/Contact person	Application Specialists +49 (0)40/ 521 00 666 AD@schuelke.com
1.4 Emergency telephone number	
	Carechem 24 International:+44 1235 239670
SECTION 2. Hazarda identificat	ion

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008) as amended by GB-CLP Regulation, UK SI 2019/720, and UK SI 2020/1567)

Eye irritation, Category 2

H319: Causes serious eye irritation.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008) as amended by GB-CLP Regulation, UK SI 2019/720, and UK SI 2020/1567)

Hazard pictograms

Hazaro pictograms	:	
Signal word	:	Warning
Hazard statements	:	H319 Causes serious eye irritation.
Precautionary statements	:	Prevention: P280 Wear eye protection/ face protection.
		Response: P305 + P351 + P338 IF IN EYES: Rinse cautiously with wa- ter for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313 If eye irritation persists: Get medical advice/ attention.

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Chemical nature

: Solution of the following substances with harmless additives.

Hazardous components

Chemical name	CAS-No.	Classification	Concentration
	EC-No.		(% w/w)
	Index-No.		
	Registration number		
1,2,3-Propanetricarboxylic acid, 2-	5949-29-1	Eye Irrit. 2; H319	>= 10 - < 20
hydroxy-, monohydrate	201-069-1	STOT SE 3; H335	
		(Respiratory sys-	
	01-2119457026-42-	tem)	
	XXXX	STOT SE 3; H335	
		(Respiratory sys-	
		tem)	
2-phosphonobutane-1,2,4-	37971-36-1	Met. Corr. 1; H290	>= 1 - < 10
tricarboxylic acid	253-733-5	Eye Irrit. 2; H319	
	01-2119436643-39-		
	XXXX		

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For explanation of abbreviations see section 16.

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice	:	Take off all contaminated clothing immediately.
If inhaled	:	If symptoms persist, call a physician.
In case of skin contact	:	Wash with water and soap as a precaution. If symptoms persist, call a physician.
In case of eye contact	:	In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice. If eye irritation persists, consult a specialist.
If swallowed	:	Rinse mouth with water. Give small amounts of water to drink. Consult a physician if necessary.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms	: Treat symptomatically.
Risks	: Causes serious eye irritation.

4.3 Indication of any immediate medical attention and special treatment needed

Treatment	: For specialist advice physicians should contact the Poisons Information Service.

SECTION 5: Firefighting measures

5.1	Extinguishing media		
	Suitable extinguishing media	:	Dry powder Foam Water spray jet Carbon dioxide (CO2)
	Unsuitable extinguishing media	:	Do NOT use water jet.
5.2	Special hazards arising from	the	substance or mixture
	Specific hazards during fire- fighting	:	No information available.
	Hazardous combustion prod- ucts	:	No hazardous combustion products are known

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5.3 Advice for firefighters

Special protective equipment : In the event of fire, wear self-contained breathing apparatus. for firefighters

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures Personal precautions : Use personal protective equipment. 6.2 Environmental precautions Environmental precautions Avoid subsoil penetration. 6.3 Methods and material for containment and cleaning up Methods for cleaning up Wipe up with absorbent material (e.g. cloth, fleece). : Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). 6.4 Reference to other sections see Section 8 + 13 **SECTION 7: Handling and storage** 7.1 Precautions for safe handling Advice on safe handling 1 Never mix concentrates directly. Advice on protection against : No special protective measures against fire required. fire and explosion Keep away from food and drink. Hygiene measures : 7.2 Conditions for safe storage, including any incompatibilities Requirements for storage : Store at room temperature in the original container. areas and containers Further information on stor-Keep away from heat. Keep container tightly closed. Recomage conditions mended storage temperature: 5 - 25°C Advice on common storage Do not store together with alkalis. :

7.3 Specific end use(s)

Specific use(s)

: none

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Contains no substances with occupational exposure limit values.

Predicted No Effect Concentration (PNEC):

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Substance name	Environmental Compartment	Value
1,2,3-Propanetricarboxylic acid,	Fresh water	0.44 mg/l
2-hydroxy-, monohydrate		-
	Marine water	0.044 mg/l
	Fresh water sediment	7.52 mg/kg
	Marine sediment	0.752 mg/kg
	Soil	29.2 mg/kg
2-phosphonobutane-1,2,4-	Fresh water	0.666 mg/l
tricarboxylic acid		
	Marine water	0.066 mg/l
	Effects on waste water treatment plants	50.4 mg/l
	Fresh water sediment	2.398 mg/kg dry
		weight (d.w.)
	Marine sediment	0.24 mg/kg dry
		weight (d.w.)
	Soil	0.089 mg/kg dry
		weight (d.w.)

8.2 Exposure controls

Personal protective equipment					
Eye/face protection Hand protection	:	Safety glasses with side-shields conforming to EN166			
Directive	:	The selected protective gloves have to satisfy the specifica- tions of Regulation (EU) 2016/425 and the standard EN 374 derived from it.			
Remarks	:	Splash protection: disposable nitrile rubber gloves e.g. Dermatril (layer thickness: 0.11 mm) made by KCL or gloves from other manufacturers offering the same protection. Pro- longed contact: Nitrile rubber gloves e.g. Camatril (>480 Min., layer thickness: 0,40 mm) or butyl rubber gloves e.g. Butoject (>480 Min., layer thickness: 0,70 mm) made by KCL or gloves from other manufacturers offering the same protec- tion.			
Skin and body protection Respiratory protection	:	Work uniform or laboratory coat. No personal respiratory protective equipment normally re-			
Protective measures	:	quired. Avoid contact with eyes.			

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance Colour Odour Odour Threshold	: : :	liquid colourless nearly odourless not determined
рН	:	1.3 (20 °C) Concentration: 100 %
Decomposition temperature	:	No data available

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Melting point/freezing point	< -5 °C	
Boiling point/boiling range	: Not applicable	
Flash point	: >100 °C	
Evaporation rate	: No data available	
Flammability (solid, gas)	: Not applicable	
Upper explosion limit / Upper flammability limit	: Not applicable	
Lower explosion limit / Lower flammability limit	: Not applicable	
Vapour pressure	: No data available	
Relative vapour density	: No data available	
Density	: ca. 1.08 g/cm3 (20 °C)	
Solubility(ies) Water solubility	: completely soluble (20 °C)	
Partition coefficient: n- octanol/water	: Not applicable	
Auto-ignition temperature	: No data available	
Viscosity Viscosity, kinematic	: not determined	
Explosive properties	: No data available	
Oxidizing properties	: The substance or mixture is not classified as oxidizing.	
9.2 Other information Metal corrosion rate	: Not corrosive to metals	

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SECTION 10: Stability and reactivity

10.1 Reactivity

No dangerous reaction known under conditions of normal use.

10.2 Chemical stability

The product is chemically stable.

10.3 Possibility of hazardous reactions

Hazardous reactions : Reaction with alkalis(caustic liquors).

10.4 Conditions to avoid

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Conditions to	avoid :	Protect from frost, heat and sunlight.		
10.5 Incompatibl Materials to a		No data available		
10.6 Hazardous decomposition products None reasonably foreseeable.				
SECTION 11: Toxicological information				
11.1 Information on toxicological effects				
Acute toxicity Not classified based on available information.				
<u>Components</u>	<u>s:</u>			
1,2,3-Propar Acute oral to:		I, 2-hydroxy-, monohydrate: LD50 (Mouse): 5,400 mg/kg Method: OECD Test Guideline 401		

Acute oral toxicity	:	LD50 (Mouse): 5,400 mg/kg Method: OECD Test Guideline 401
Acute inhalation toxicity	:	Remarks: No data available
Acute dermal toxicity	:	LD50 (Rat): > 2,000 mg/kg
Acute toxicity (other routes of administration)	:	LD50 intravenous (Rat): 725 mg/kg

2-phosphonobutane-1,2,4-tricarboxylic acid:

		<i>y</i>
Acute oral toxicity	:	LD50 (Rat): > 2,000 mg/kg Method: EC Directive 92/69/EEC B.1 Acute Toxicity (Oral) Remarks: Based on data from similar materials
Acute inhalation toxicity	:	LC50 (Rat): > 1.979 mg/l Exposure time: 4 h Test atmosphere: dust/mist Method: OECD Test Guideline 403 Assessment: An LC50/inhalation/4h/rat could not be deter- mined because no mortality of rats was observed at the max- imum achievable concentration., The substance or mixture has no acute inhalation toxicity Remarks: Based on data from similar materials
Acute dermal toxicity	:	LD50 (Rat, male and female): > 4,000 mg/kg Remarks: Based on data from similar materials

Skin corrosion/irritation

Not classified based on available information.

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Species : Rabbit

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Result	:	Mild skin irritation
Remarks	:	Based on available data, the classification criteria are not met.
2-phosphon	obutane-1,2,4-trica	arboxylic acid:
Species	:	reconstructed human epidermis (RhE)
Method	:	OECD Test Guideline 431
Result	:	No skin irritation
GLP	:	yes
Serious eye	damage/eye irritat	tion
•	ous eye irritation.	
Product:		
Remarks	:	Causes serious eye irritation.
<u>Components</u>	<u>s:</u>	
1,2,3-Propar	netricarboxylic acid	d, 2-hydroxy-, monohydrate:
Species	:	Rabbit
Method	:	OECD Test Guideline 405
Result	:	Eye irritation
2-phosphon	obutane-1,2,4-trica	arboxylic acid:
Method	:	in vitro eye irritation test
	•	

Result : Eye irritation GLP : yes

Respiratory or skin sensitisation

Skin sensitisation

Not classified based on available information.

Respiratory sensitisation

Not classified based on available information.

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Method Result	:	OECD Test Guideline 406
Result	:	Does not cause skin sensitisation.

2-phosphonobutane-1,2,4-tricarboxylic acid:

Test Type	:	Maximisation Test
Exposure routes	:	Skin contact
Species	:	Guinea pig
Method	:	OECD Test Guideline 406
Result	:	Does not cause skin sensitisation.
Test Type Exposure routes Species Method Result Remarks	:	Based on data from similar materials

Germ cell mutagenicity

Not classified based on available information.

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Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Genotoxicity in vitro	:	Test Type: Ames test Test system: Salmonella typhimurium Concentration: 0 - 5 mg/ plate Method: Mutagenicity (Salmonella typhimurium - reverse mu- tation assay) Result: negative
		Test Type: Micronucleus test Test system: Human lymphocytes Method: Mutagenicity (in vitro mammalian cytogenetic test) Result: positive
Genotoxicity in vivo	:	Species: Rat Application Route: Oral Method: OECD Test Guideline 475 Result: negative
Germ cell mutagenicity- As- sessment	:	In vitro tests did not show mutagenic effects

2-phosphonobutane-1,2,4-tricarboxylic acid:

Genotoxicity in vitro	: Test Type: Chromosome aberration test in vitro Test system: Chinese hamster lung cells Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476 Result: negative

Carcinogenicity

Not classified based on available information.

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Carcinogenicity - Assess-	:	Not classifiable as a human carcinogen.
ment		

2-phosphonobutane-1,2,4-tricarboxylic acid:

Remarks

: This information is not available.

Reproductive toxicity

Not classified based on available information.

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Effects on foetal develop- ment	:	Species: Rat Application Route: Oral General Toxicity Maternal: NOAEL: 2,500 mg/kg body weight
Reproductive toxicity - As- sessment	:	No toxicity to reproduction

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2-phosphonobutane-1,2,4-tricarboxylic acid:

Effects on foetal develop- ment	 Test Type: Pre-natal Species: Rat, female Application Route: Oral General Toxicity Maternal: NOAEL: >= 1,000 mg/kg body weight Teratogenicity: NOAEL: >= 1,000 mg/kg body weight Developmental Toxicity: NOAEL: >= 1,000 mg/kg body weight Embryo-foetal toxicity: NOAEL: >= 1,000 mg/kg body weight Method: OECD Test Guideline 414 Result: No teratogenic effects

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STOT - single exposure

Not classified based on available information.

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Exposure routes	:	Inhalation
Assessment	:	May cause respiratory irritation.

2-phosphonobutane-1,2,4-tricarboxylic acid:

Remarks :

STOT - repeated exposure

Not classified based on available information.

Components:

Remarks

: No data available

2-phosphonobutane-1,2,4-tricarboxylic acid:

Remarks	:	No data available
---------	---	-------------------

Repeated dose toxicity

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Species	:	Rat
NOAEL	:	4,000 mg/kg
LOAEL	:	8,000 mg/kg
Application Route	:	Oral
Exposure time	:	10 d

2-phosphonobutane-1,2,4-tricarboxylic acid:

Species NOAEL	:	Rat, male and female
NOAEL	:	424 mg/kg

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E	Application Route Exposure time Jumber of exposures Dose Method Remarks	:	Oral 90-day 7 Tage/ Woche 5000 ppm OECD Test Guideline 408
			•
	Jose		
Ν	lethod	:	OECD Test Guideline 408
F	Remarks	:	Subchronic toxicity
			Based on data from similar materials

Aspiration toxicity

Not classified based on available information.

Experience with human exposure

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Inhalation	:	Target Organs: respiratory tract irritation

Further information

Product:

Remarks : No data available

SECTION 12: Ecological information

12.1 Toxicity

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:				
Toxicity to fish	:	LC50 (Leuciscus idus (Golden orfe)): 440 - 760 mg/l Exposure time: 96 h		
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna): 85 - 120 mg/l Exposure time: 72 h		
Toxicity to algae/aquatic plants	:	NOEC (Scenedesmus quadricauda (Green algae)): 425 mg/l Exposure time: 8 Days Test Type: static test		
Toxicity to microorganisms	:	(Pseudomonas putida): > 10,000 mg/l Exposure time: 16 h		
2-nhosnhonohutane-1 2 4-tricarboxylic acid:				

2-phosphonobutane-1,2,4-tricarboxylic acid:

Toxicity to fish (Chronic tox-	:	> 1,042 mg/l
icity)		Exposure time: 14 d
		Species: Danio rerio (zebra fish)
		Method: OECD Test Guideline 204

12.2 Persistence and degradability

Product:

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Biodegrad	dability :	Result: Readily biodegradable. Method: OECD 301D / EEC 84/449 C6
Compone	ents:	
1,2,3-Pro	panetricarboxylic aci	d, 2-hydroxy-, monohydrate:
Biodegrad	dability :	Result: Readily biodegradable. Biodegradation: 97 % Exposure time: 28 d Method: OECD Test Guideline 301B
2-phosph	nonobutane-1,2,4-trica	arboxylic acid:
Biodegrad	dability :	Test Type: aerobic Result: Not rapidly biodegradable Biodegradation: 0 % Exposure time: 28 d Method: OECD Test Guideline 301E
12.3 Bioaccu	mulative potential	
Compone	ents:	
1, 2,3-Pro Bioaccum		 d, 2-hydroxy-, monohydrate: Remarks: No bioaccumulation is to be expected (log Pow <= 4).
2-phospł	nonobutane-1,2,4-trica	arboxylic acid:
Bioaccum	iulation :	Remarks: No data available

: log Pow: -1.36 (25 °C)
Method: calculated

12.4 Mobility in soil

Components:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, monohydrate:

Mobility : Remarks: No data available

2-phosphonobutane-1,2,4-tricarboxylic acid:

Mobility : Remarks: No data available

12.5 Results of PBT and vPvB assessment

Product:

Assessment	:	This substance/mixture contains no components considered
		to be either persistent, bioaccumulative and toxic (PBT), or
		very persistent and very bioaccumulative (vPvB) at levels of
		0.1% or higher.

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12.6 Other adverse effects

Product:

Endocrine disrupting poten- tial	:	The substance/mixture does not contain components consid- ered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Additional ecological infor- mation	:	No data is available on the product itself.

SECTION 13: Disposal considerations

13.1 Waste treatment methods		
Product	:	Disposal together with normal waste is not allowed. Special disposal required according to local regulations.
Contaminated packaging	:	Empty containers should be taken to an approved waste han- dling site for recycling or disposal.

SECTION 14: Transport information

14.1 UN number

ADR	:	Not regulated as a dangerous good
IMDG	:	Not regulated as a dangerous good
ΙΑΤΑ	:	Not regulated as a dangerous good
14.2 UN proper shipping name		
ADR	:	Not regulated as a dangerous good
IMDG	:	Not regulated as a dangerous good
ΙΑΤΑ	:	Not regulated as a dangerous good
14.3 Transport hazard class(es)		
ADR	:	Not regulated as a dangerous good
IMDG	:	Not regulated as a dangerous good
ΙΑΤΑ	:	Not regulated as a dangerous good
14.4 Packing group		
ADR	:	Not regulated as a dangerous good
IMDG	:	Not regulated as a dangerous good
IATA (Cargo)	:	Not regulated as a dangerous good
IATA (Passenger)	:	Not regulated as a dangerous good
14.5 Environmental hazards		

Not regulated as a dangerous good

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14.6 Special precautions for user

Not applicable

14.7 Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable for product as supplied.

SECTION 15: Regulatory information

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

Relevant EU provisions transposed through retained EU law

UK REACH List of restrictions (Annex 17)	: Conditions of restriction for the fol- lowing entries should be considere Number on list 3	
UK REACH Candidate list of substances of very high concern (SVHC) for Authorisation	: Not applicable	
The Persistent Organic Pollutants Regulations (retained Regulation (EU) 2019/1021 as amended for Great Britain)	: Not applicable	
Regulation (EC) on substances that deplete the ozone layer	: Not applicable	
UK REACH List of substances subject to authorisation (Annex XIV)	: Not applicable	
	of 24 November 2010 on industrial	

emissions (integrated pollution prevention and control) Volatile organic compounds (VOC) content: 0.6 %

The components of this product are reported in the following inventories:

TCSI	:	On the inventory, or in compliance with the inventory
TSCA	:	All substances listed as active on the TSCA inventory
AIIC	:	On the inventory, or in compliance with the inventory
DSL	:	All components of this product are on the Canadian DSL
ENCS	:	On the inventory, or in compliance with the inventory
ISHL	:	On the inventory, or in compliance with the inventory
KECI	:	On the inventory, or in compliance with the inventory
PICCS	:	On the inventory, or in compliance with the inventory
IECSC	:	On the inventory, or in compliance with the inventory
NZIoC	:	Not in compliance with the inventory
TECI	:	On the inventory, or in compliance with the inventory

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15.2 Chemical safety assessment

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

SECTION 16: Other information

Full text of H-Statements

H290	:	May be corrosive to metals.
H319	:	Causes serious eye irritation.
H335	:	May cause respiratory irritation.

Full text of other abbreviations

Eye Irrit. :	Eye irritation
Met. Corr. :	Corrosive to metals
STOT SE :	Specific target organ toxicity - single exposure

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CLP - Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECHA -European Chemicals Agency; EC-Number - European Community number; ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergencv Schedule: ENCS - Existing and New Chemical Substances (Japan): ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; SVHC - Substance of very high concern; TCSI - Taiwan Chemical Substance Inventory; TECI -Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Further information			
Classification of the mixture:			
Eye Irrit. 2	H319		

Classification procedure: Calculation method

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Changes since the last version are highlighted in the margin. This version replaces all previous versions.

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