

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830
Date of issue: 10/11/2019 Version: 1.0

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

1.1. Product identifier

Product form	: Mixture
Product name	: Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)
CAS-No.	: 27668-52-6
Product code	: 27361129
Formula	: C26H58ClNO3Si
Product group	: Blend

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

1.2.1. Relevant identified uses

Main use category	: Laboratory use, Industrial use, Professional use
Industrial/Professional use spec	: For professional use only
Use of the substance/mixture	: For analytical purposes Scientific research and development Not for human consumption or veterinary purposes.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Scafell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

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

Flammable liquids, Category 2	H225
Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Hazardous to the aquatic environment — Acute Hazard, Category 1	H400
Full text of H statements : see section 16	

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

GHS02

GHS09

Signal word (CLP) :

Danger

Hazardous ingredients :

Isopropanol (Propan-2-ol)

Hazard statements (CLP) :

H225 - Highly flammable liquid and vapour.
H315 - Causes skin irritation.
H319 - Causes serious eye irritation.
H400 - Very toxic to aquatic life.

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Precautionary statements (CLP) : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P264 - Wash hands, forearms and face thoroughly after handling.
P273 - Avoid release to the environment.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Not applicable

3.2. Mixtures

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride	(CAS-No.) 27668-52-6 (EC-No.) 248-595-8	55 - 65	Skin Irrit. 2, H315 Eye Irrit. 2, H319 Aquatic Acute 1, H400
Isopropanol (Propan-2-ol)	(CAS-No.) 67-63-0 (EC-No.) 200-661-7 (EC Index-No.) 603-117-00-0	35 - 45	Flam. Liq. 2, H225 Eye Irrit. 2, H319 STOT SE 3, H336

Full text of H-statements: see section 16

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.

First-aid measures after inhalation : If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.

First-aid measures after skin contact : After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.

First-aid measures after eye contact : Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.

First-aid measures after ingestion : Rinse mouth out with water. Do not induce vomiting. Get medical advice/attention.

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

Symptoms/effects after inhalation : Inhalation may cause irritation (cough, short breathing, difficulty in breathing).

Symptoms/effects after skin contact : Causes skin irritation. Itching. Redness, pain.

Symptoms/effects after eye contact : Causes serious eye irritation. redness, itching, tears.

Symptoms/effects after ingestion : Ingestion may cause nausea, vomiting and diarrhea.

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

Get immediate medical advice/attention.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Dry powder. Sand. Water spray. Carbon dioxide. Foam.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Flammable liquid and vapour.

Explosion hazard : May form flammable/explosive vapour-air mixture.

Hazardous decomposition products in case of fire : irritating vapours are released.

5.3. Advice for firefighters

Precautionary measures fire : Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.

Firefighting instructions : Exercise caution when fighting any chemical fire. Use water spray or fog for cooling exposed containers. Prevent fire fighting water from entering the environment.

Protection during firefighting : Wear recommended personal protective equipment. Use self-contained breathing apparatus and chemically protective clothing.

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Other information : Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Do not handle until all safety precautions have been read and understood. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc). Keep away from combustible materials.

6.1.1. For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.

Emergency procedures : Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.

Measures in case of dust release : Shelter from vapours by keeping upwind. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc). Special attention should be given to low areas/pits where flammable vapours can accumulate.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use self-contained breathing apparatus and chemically protective clothing.

Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Collect spillage. Contain the spilled material by bunding.

Methods for cleaning up : Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible. Try to stop release if without risk.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapours are flammable.

Precautions for safe handling : Avoid formation of vapours. Avoid contact with skin, eyes and clothing. Do not handle until all safety precautions have been read and understood. Ensure that there is a suitable ventilation system. Do not handle in a confined space.

Hygiene measures : Take off immediately all contaminated clothing and wash it before reuse. Contaminated work clothing should not be allowed out of the workplace. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ensure adequate ventilation, especially in confined areas. Proper grounding procedures to avoid static electricity should be followed.

Storage conditions : Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use.

Incompatible products : Strong oxidizing agents. Alkali metals. Strong acids. Acid chlorides. Acid anhydrides. reducing agents.

Incompatible materials : Sources of ignition. Direct sunlight. Heat sources. open flames. sparks.

Heat and ignition sources : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Storage area : Keep away from combustible materials. Store below 20 °C. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

For analytical purposes. Scientific research and development. Not for human consumption or veterinary purposes.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution) (27668-52-6)

Country	Local name	Value
United Kingdom	Local name	Propan-2-ol
United Kingdom	WEL TWA (mg/m ³)	999 mg/m ³
United Kingdom	WEL TWA (ppm)	400 ppm
United Kingdom	WEL STEL (mg/m ³)	1250 mg/m ³

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Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution) (27668-52-6)		
United Kingdom	WEL STEL (ppm)	500 ppm
United Kingdom	Regulatory reference	EH40/2005 (Third edition, 2018). HSE
Isopropanol (Propan-2-ol) (67-63-0)		
United Kingdom	Local name	Propan-2-ol
United Kingdom	WEL TWA (mg/m ³)	999 mg/m ³
United Kingdom	WEL TWA (ppm)	400 ppm
United Kingdom	WEL STEL (mg/m ³)	1250 mg/m ³
United Kingdom	WEL STEL (ppm)	500 ppm
United Kingdom	Regulatory reference	EH40/2005 (Third edition, 2018). HSE

8.2. Exposure controls

Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures. Floors should be impervious, resistant to liquids and easy to clean.

Personal protective equipment:

Avoid all unnecessary exposure.

Materials for protective clothing:

Wear suitable protective clothing, gloves and eye/face protection

Hand protection:

The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374

Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Fluoroelastomer (FKM)	6 (> 480 minutes)	0.7		EN 374

Eye protection:

Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against liquid splashes.

Type	Use	Characteristics	Standard
Safety goggles, Face shield	Droplet, vapours	tightly fitting safety goggles, With side shields	EN 166

Skin and body protection:

Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use

Type	Standard
Total impervious protective suits, gloves, and boots must be worn to prevent any contact with the product, Flame retardant antistatic protective clothing	EN 14605

Respiratory protection:

Keep self contained breathing apparatus readily available for emergency use. Where exposure through inhalation may occur from use, respiratory protection equipment is recommended

Device	Filter type	Condition	Standard
Air-Purifying Respirator (APR), reusable	ABEK	Moist condition, Mist formation, Protection for Liquid particles, Vapour protection	EN 14387

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Liquid
Molecular mass : 496.28 g/mol

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Colour	: light yellow. amber. light brown.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: No data available
Flash point	: 11 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Flammable
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: 0.89 g/mL
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Flammable liquid and vapour.

10.2. Chemical stability

Flammable liquid and vapour. May form flammable/explosive vapour-air mixture.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5. Incompatible materials

Strong oxidizers. Alkali metals. Strong acids. Acid chlorides. Acid anhydrides. reducing agents.

10.6. Hazardous decomposition products

No hazardous decomposition products known at room temperature. Thermal decomposition generates : irritating vapours.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (27668-52-6)

LD50 oral rat	> 5000 mg/kg
LD50 dermal rat	> 2000 mg/kg
LC50 inhalation rat (mg/l)	> 2 mg/l 1hr

Isopropanol (Propan-2-ol) (67-63-0)

LD50 oral rat	5045 mg/kg
LD50 dermal rabbit	12800 mg/kg
LC50 inhalation rat (ppm)	10000 ppm 6h
LC50 inhalation rat (Vapours - mg/l/4h)	37.5 mg/l/4h

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

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Serious eye damage/irritation	: Causes serious eye irritation.
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity	: Very toxic to aquatic life.
Chronic aquatic toxicity	: Not classified

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (27668-52-6)

LC50 fish 1	510 µg/l <i>Lepomis macrochirus</i> (Bluegill) 96hr
LC50 fish 2	560 µg/l <i>Oncorhynchus mykiss</i> (Rainbow Trout) 96hr
EC50 Daphnia 1	720 µg/l <i>Daphnia magna</i> (Water Flea) 48hr

Isopropanol (Propan-2-ol) (67-63-0)

LC50 fish 1	9640 mg/l <i>Pimephales promelas</i> (fathead minnow) - 96h
EC50 Daphnia 1	13299 mg/l <i>Daphnia magna</i> (Water flea) - 48h

12.2. Persistence and degradability

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution) (27668-52-6)

Persistence and degradability	No data available.
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Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (27668-52-6)

Persistence and degradability	No data available.
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Isopropanol (Propan-2-ol) (67-63-0)

Persistence and degradability	No data available.
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12.3. Bioaccumulative potential

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution) (27668-52-6)

Bioaccumulative potential	No data available.
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Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (27668-52-6)

Log Pow	4.9 (est)
Bioaccumulative potential	No data available.

Isopropanol (Propan-2-ol) (67-63-0)

Log Pow	0.05
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Bioaccumulative potential	No data available.
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12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution) (27668-52-6)

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

Component

Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (27668-52-6)	This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII
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12.6. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods






Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Additional information : Handle empty containers with care because residual vapours are flammable.

Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
1993	1993	1993	1993	1993
14.2. UN proper shipping name				
FLAMMABLE LIQUID, N.O.S.	FLAMMABLE LIQUID, N.O.S.	Flammable liquid, n.o.s.	FLAMMABLE LIQUID, N.O.S.	FLAMMABLE LIQUID, N.O.S.
Transport document description				
UN 1993 FLAMMABLE LIQUID, N.O.S. (Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)), 3, II, (D/E), ENVIRONMENTALLY HAZARDOUS	UN 1993 FLAMMABLE LIQUID, N.O.S. (Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)), 3, II, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS	UN 1993 Flammable liquid, n.o.s. (Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)), 3, II, ENVIRONMENTALLY HAZARDOUS	UN 1993 FLAMMABLE LIQUID, N.O.S. (Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)), 3, II, ENVIRONMENTALLY HAZARDOUS	UN 1993 FLAMMABLE LIQUID, N.O.S. (Dimethyloctadecyl[3-(trimethoxysilyl)propyl]ammonium chloride (60% in IPA solution)), 3, II, ENVIRONMENTALLY HAZARDOUS
14.3. Transport hazard class(es)				
3	3	3	3	3
				
14.4. Packing group				
II	II	II	II	II
14.5. Environmental hazards				
Dangerous for the environment : Yes	Dangerous for the environment : Yes Marine pollutant : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes

No supplementary information available

14.6. Special precautions for user

Overland transport

Classification code (ADR) : F1

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Special provisions (ADR)	: 274, 601, 640D
Limited quantities (ADR)	: 1I
Excepted quantities (ADR)	: E2
Packing instructions (ADR)	: P001, IBC02, R001
Mixed packing provisions (ADR)	: MP19
Portable tank and bulk container instructions (ADR)	: T7
Portable tank and bulk container special provisions (ADR)	: TP1, TP8, TP28
Tank code (ADR)	: LGBF
Vehicle for tank carriage	: FL
Transport category (ADR)	: 2
Special provisions for carriage - Operation (ADR)	: S2, S20
Hazard identification number (Kemler No.)	: 33
Orange plates	:



Tunnel restriction code (ADR)	: D/E
EAC code	: •3YE

Transport by sea

Special provisions (IMDG)	: 274
Limited quantities (IMDG)	: 1 L
Excepted quantities (IMDG)	: E2
Packing instructions (IMDG)	: P001
IBC packing instructions (IMDG)	: IBC02
Tank instructions (IMDG)	: T7
Tank special provisions (IMDG)	: TP1, TP28, TP8
EmS-No. (Fire)	: F-E
EmS-No. (Spillage)	: S-E
Stowage category (IMDG)	: B

Air transport

PCA Excepted quantities (IATA)	: E2
PCA Limited quantities (IATA)	: Y341
PCA limited quantity max net quantity (IATA)	: 1L
PCA packing instructions (IATA)	: 353
PCA max net quantity (IATA)	: 5L
CAO packing instructions (IATA)	: 364
CAO max net quantity (IATA)	: 60L
Special provisions (IATA)	: A3
ERG code (IATA)	: 3H

Inland waterway transport

Classification code (ADN)	: F1
Special provisions (ADN)	: 274, 601, 640C
Limited quantities (ADN)	: 1 L
Excepted quantities (ADN)	: E2
Carriage permitted (ADN)	: T
Equipment required (ADN)	: PP, EX, A
Ventilation (ADN)	: VE01
Number of blue cones/lights (ADN)	: 1

Rail transport

Classification code (RID)	: F1
Special provisions (RID)	: 274, 601, 640C
Limited quantities (RID)	: 1L
Excepted quantities (RID)	: E2
Packing instructions (RID)	: P001
Mixed packing provisions (RID)	: MP19

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Portable tank and bulk container instructions (RID)	: T7
Portable tank and bulk container special provisions (RID)	: TP1, TP8, TP28
Tank codes for RID tanks (RID)	: L1.5BN
Transport category (RID)	: 2
Colis express (express parcels) (RID)	: CE7
Hazard identification number (RID)	: 33

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

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

Contains no REACH substances with Annex XVII restrictions
Contains no substance on the REACH candidate list
Contains no REACH Annex XIV substances
Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

Full text of H- and EUH-statements:	
Aquatic Acute 1	Hazardous to the aquatic environment — Acute Hazard, Category 1
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Flam. Liq. 2	Flammable liquids, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Narcosis
H225	Highly flammable liquid and vapour.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.