

# 2,2,4-TRIMETHYLPENTANE FOR HPLC & UV SPECTROSCOPY

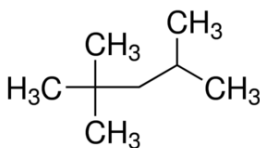
## Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878  
Reference number: 00352  
Issue date: 4/10/2024 Revision date: 4/10/2024 Supersedes version of: 4/16/2016 Version: 1.0

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

#### 1.1. Product identifier

Product form : Substance  
Trade name : 2,2,4-TRIMETHYLPENTANE FOR HPLC & UV SPECTROSCOPY  
EC Index-No. : 601-009-00-8  
EC-No. : 208-759-1  
CAS-No. : 540-84-1  
Product code : 00352  
Type of product : Hydrocarbons, aliphatic  
Formula : C<sub>8</sub>H<sub>18</sub>  
Chemical structure :



Synonyms : iso-Octane

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

##### 1.2.1. Relevant identified uses

Industrial/Professional use spec : Industrial  
For professional use only  
Use of the substance/mixture : Laboratory chemicals  
Manufacture of substances  
Solvents

##### 1.2.2. Uses advised against

No additional information available

#### 1.3. Details of the supplier of the safety data sheet

LOBA CHEMIE PVT.LTD.  
107 Wode House Road, Jehangir Villa, Colaba  
400005 Mumbai  
INDIA  
T +91 22 6663 6663, F +91 22 6663 6699  
[info@lobachemie.com](mailto:info@lobachemie.com), [www.lobachemie.com](http://www.lobachemie.com)

#### 1.4. Emergency telephone number

Emergency number : + 91 22 6663 6663 (9:00am - 6:00 pm)

### 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
Specific target organ toxicity – Single exposure, Category 3, Narcosis	H336
Aspiration hazard, Category 1	H304
Hazardous to the aquatic environment – Acute Hazard, Category 1	H400
Hazardous to the aquatic environment – Chronic Hazard, Category 1	H410

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

### Adverse physicochemical, human health and environmental effects

Highly flammable liquid and vapour. May cause drowsiness or dizziness. Causes skin irritation. May be fatal if swallowed and enters airways. Very toxic to aquatic life with long lasting effects.

## 2.2. Label elements

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

Hazard pictograms (CLP)



Signal word (CLP)

Hazard statements (CLP)

Precautionary statements (CLP)

- : Danger
- : H225 - Highly flammable liquid and vapour.
- : H304 - May be fatal if swallowed and enters airways.
- : H315 - Causes skin irritation.
- : H336 - May cause drowsiness or dizziness.
- : H410 - Very toxic to aquatic life with long lasting effects.
- : 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.
- : P273 - Avoid release to the environment.
- : P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor.
- : P303+P361+P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water .
- : P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.

## 2.3. Other hazards

Contains no PBT and/or vPvB substances  $\geq 0.1\%$  assessed in accordance with REACH Annex XIII

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Substance type

: Mono-constituent

Name	Product identifier	%
2,2,4-TRIMETHYLPENTANE	CAS-No.: 540-84-1 EC-No.: 208-759-1 EC Index-No.: 601-009-00-8	100

### 3.2. Mixtures

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general

First-aid measures after inhalation

First-aid measures after skin contact

First-aid measures after eye contact

- : Call a physician immediately.
- : Remove person to fresh air and keep comfortable for breathing. Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
- : Wash with plenty of water/... Wash contaminated clothing before reuse. Get medical advice/attention. Rinse skin with water/shower. Take off immediately all contaminated clothing. If skin irritation occurs: Get medical advice/attention.
- : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

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First-aid measures after ingestion : Immediately call a POISON CENTER/doctor. Rinse mouth. Do not induce vomiting. Call a physician immediately.

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

Symptoms/effects : May cause drowsiness or dizziness.  
Symptoms/effects after inhalation : May cause drowsiness or dizziness.  
Symptoms/effects after skin contact : Causes skin irritation. Irritation.  
Symptoms/effects after eye contact : None under normal conditions.  
Symptoms/effects after ingestion : May be fatal if swallowed and enters airways. Risk of lung oedema.

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide. Dry powder. Foam. Water spray.  
Unsuitable extinguishing media : Do not use extinguishing media containing water.

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

Fire hazard : Highly flammable liquid and vapour.  
Explosion hazard : May form flammable/explosive vapour-air mixture.  
Hazardous decomposition products in case of fire : Toxic fumes may be released.

### 5.3. Advice for firefighters

Firefighting instructions : Fight fire from safe distance and protected location. Do not enter fire area without proper protective equipment, including respiratory protection.  
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

## SECTION 6: Accidental release measures

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

General measures : Remove ignition sources. Use special care to avoid static electric charges. No open flames. No smoking. Stop leak if safe to do so. Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material damage.

#### 6.1.1. For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.  
Emergency procedures : Ventilate spillage area. Evacuate unnecessary personnel. No open flames, no sparks, and no smoking. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid contact with skin and eyes.

#### 6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use personal protective equipment as required. For further information refer to section 8: "Exposure controls/personal protection".  
Emergency procedures : Ventilate area. Evacuate unnecessary personnel. Stop leak if safe to do so.

### 6.2. Environmental precautions

Avoid release to the environment. Very toxic to aquatic life with long lasting effects.

### 6.3. Methods and material for containment and cleaning up

For containment : Collect spillage. Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams. Stop leak without risks if possible.

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- Methods for cleaning up : Take up liquid spill into absorbent material. On land, sweep or shovel into suitable containers. Collect spillage. Notify authorities if product enters sewers or public waters.
- Other information : Dispose of materials or solid residues at an authorized site.

### 6.4. Reference to other sections

For further information refer to section 13.

## 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 : Keep away from sources of ignition - No smoking. Do not breathe vapours. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Flammable vapours may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Use only outdoors or in a well-ventilated area. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid contact with skin and eyes.
- Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

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

- Technical measures : Proper grounding procedures to avoid static electricity should be followed. Ground/bond container and receiving equipment.
- Storage conditions : Keep in fireproof place. Store in a well-ventilated place. Keep cool. Keep container tightly closed. Store locked up.
- Incompatible materials : Heat sources.
- Packaging materials : Store always product in container of same material as original container.

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### 8.1.1 National occupational exposure and biological limit values

No additional information available

#### 8.1.2. Recommended monitoring procedures

No additional information available

#### 8.1.3. Air contaminants formed

No additional information available

#### 8.1.4. DNEL and PNEC

No additional information available

#### 8.1.5. Control banding

No additional information available

### 8.2. Exposure controls

#### 8.2.1. Appropriate engineering controls

**Appropriate engineering controls:**

Ensure good ventilation of the work station.

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### 8.2.2. Personal protection equipment

#### Personal protective equipment:

Wear recommended personal protective equipment.

#### Personal protective equipment symbol(s):



#### 8.2.2.1. Eye and face protection

##### Eye protection:

Chemical goggles or safety glasses

#### 8.2.2.2. Skin protection

##### Skin and body protection:

Wear a mask

##### Hand protection:

Protective gloves

#### 8.2.2.3. Respiratory protection

##### Respiratory protection:

Wear appropriate mask

#### 8.2.2.4. Thermal hazards

No additional information available

### 8.2.3. Environmental exposure controls

#### Environmental exposure controls:

Avoid release to the environment.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Colour	: Colourless.
Appearance	: Clear liquid.
Molecular mass	: 114.23 g/mol
Odour	: benzene-like, petroleum-like odour.
Odour threshold	: Not available
Melting point	: Not applicable
Freezing point	: -107 °C
Boiling point	: 98 – 99 °C
Flammability	: Flammable Highly flammable liquid and vapour.
Lower explosion limit	: 1.1 vol %
Upper explosion limit	: 6 vol %
Flash point	: -12 °C
Auto-ignition temperature	: 418 °C
Decomposition temperature	: Not available
pH	: Not available
Viscosity, kinematic	: 0.737 mm <sup>2</sup> /s
Viscosity, dynamic	: 0.51 mPa·s at 22°C
Solubility	: Water: Immiscible
Partition coefficient n-octanol/water (Log Kow)	: Not available
Partition coefficient n-octanol/water (Log Pow)	: 4.6
Vapour pressure	: 5.1 kPa at 20°C
Vapour pressure at 50°C	: Not available
Density	: 0.692 g/cm <sup>3</sup> at 20°C

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Relative density : 0.69  
Relative vapour density at 20°C : 3.93 (Air = 1)  
Particle characteristics : Not applicable

### 9.2. Other information

#### 9.2.1. Information with regard to physical hazard classes

No additional information available

#### 9.2.2. Other safety characteristics

Refractive index : 1.39 – 1.392 (20 °C, 589 nm)

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Highly flammable liquid and vapour.

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

### 10.4. Conditions to avoid

Open flame. Sparks. Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

### 10.5. Incompatible materials

No additional information available

### 10.6. Hazardous decomposition products

May release flammable gases.

## SECTION 11: Toxicological information

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

Acute toxicity (oral) : Not classified  
Acute toxicity (dermal) : Not classified  
Acute toxicity (inhalation) : Not classified  
Skin corrosion/irritation : Causes skin irritation.  
Serious eye damage/irritation : Not classified  
Respiratory or skin sensitisation : Not classified  
Germ cell mutagenicity : Not classified  
Carcinogenicity : Not classified  
Reproductive toxicity : Not classified  
STOT-single exposure : May cause drowsiness or dizziness.  
STOT-repeated exposure : Not classified  
Aspiration hazard : May be fatal if swallowed and enters airways.

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Viscosity, kinematic	0.737 mm <sup>2</sup> /s
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### 11.2. Information on other hazards

No additional information available

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### SECTION 12: Ecological information

#### 12.1. Toxicity

Ecology - general	: Very toxic to aquatic life with long lasting effects.
Ecology - water	: Very toxic to aquatic life with long lasting effects.
Hazardous to the aquatic environment, short-term (acute)	: Very toxic to aquatic life.
Hazardous to the aquatic environment, long-term (chronic)	: Very toxic to aquatic life with long lasting effects.

#### 12.2. Persistence and degradability

##### 2,2,4-TRIMETHYLPENTANE FOR HPLC & UV SPECTROSCOPY (540-84-1)

Persistence and degradability	Rapidly degradable
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#### 12.3. Bioaccumulative potential

No additional information available

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Results of PBT and vPvB assessment

No additional information available

#### 12.6. Endocrine disrupting properties

No additional information available

#### 12.7. Other adverse effects

No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Regional waste regulation	: Disposal must be done according to official regulations.
Waste treatment methods	: Dispose of contents/container in accordance with licensed collector's sorting instructions.
Sewage disposal recommendations	: Disposal must be done according to official regulations.
Product/Packaging disposal recommendations	: Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation. Disposal must be done according to official regulations.
Additional information	: Handle empty containers with care because residual vapours are flammable. Flammable vapours may accumulate in the container. Do not re-use empty containers.
Ecological information	: Hazardous waste due to toxicity.

### SECTION 14: Transport information

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

#### 14.1. UN number or ID number

UN-No. (ADR)	: UN 1262
UN-No. (IMDG)	: UN 1262
UN-No. (IATA)	: UN 1262
UN-No. (ADN)	: UN 1262
UN-No. (RID)	: UN 1262

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### 14.2. UN proper shipping name

Proper Shipping Name (ADR)	: OCTANES
Proper Shipping Name (IMDG)	: OCTANES
Proper Shipping Name (IATA)	: Octanes
Proper Shipping Name (ADN)	: OCTANES
Proper Shipping Name (RID)	: OCTANES
Transport document description (ADR)	: UN 1262 OCTANES, 3, II, (D/E)
Transport document description (IMDG)	: UN 1262 OCTANES, 3, II, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS
Transport document description (IATA)	: UN 1262 Octanes, 3, II, ENVIRONMENTALLY HAZARDOUS
Transport document description (ADN)	: UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS
Transport document description (RID)	: UN 1262 OCTANES, 3, II, ENVIRONMENTALLY HAZARDOUS

### 14.3. Transport hazard class(es)

#### ADR

Transport hazard class(es) (ADR) : 3  
Danger labels (ADR) : 3



#### IMDG

Transport hazard class(es) (IMDG) : 3  
Danger labels (IMDG) : 3



#### IATA

Transport hazard class(es) (IATA) : 3  
Danger labels (IATA) : 3



#### ADN

Transport hazard class(es) (ADN) : 3  
Danger labels (ADN) : 3



#### RID

Transport hazard class(es) (RID) : 3  
Danger labels (RID) : 3



### 14.4. Packing group

Packing group (ADR) : II  
Packing group (IMDG) : II  
Packing group (IATA) : II



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Packing group (ADN) : II  
Packing group (RID) : II

### 14.5. Environmental hazards

Dangerous for the environment : Yes  
Marine pollutant : Yes  
Other information : No supplementary information available

### 14.6. Special precautions for user

#### Overland transport

Classification code (ADR) : F1  
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) : T4  
Portable tank and bulk container special provisions (ADR) : TP1  
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

Limited quantities (IMDG) : 1 L  
Excepted quantities (IMDG) : E2  
Packing instructions (IMDG) : P001  
IBC packing instructions (IMDG) : IBC02  
Tank instructions (IMDG) : T4  
Tank special provisions (IMDG) : TP2  
EmS-No. (Fire) : F-E  
EmS-No. (Spillage) : S-E  
Stowage category (IMDG) : B  
Properties and observations (IMDG) : Colourless liquids. Explosive limits: 1% to 6.5%. ISOCTANE: flashpoint-12°C c.c. n-OCTANE: flashpoint 13°C c.c. Immiscible with water.  
MFAG-No : 128

#### 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  
ERG code (IATA) : 3H

#### Inland waterway transport

Classification code (ADN) : F1  
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

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### Rail transport

Classification code (RID)	: F1
Limited quantities (RID)	: 1L
Excepted quantities (RID)	: E2
Packing instructions (RID)	: P001, IBC02, R001
Mixed packing provisions (RID)	: MP19
Portable tank and bulk container instructions (RID)	: T4
Portable tank and bulk container special provisions (RID)	: TP1
Tank codes for RID tanks (RID)	: LGBF
Transport category (RID)	: 2
Colis express (express parcels) (RID)	: CE7
Hazard identification number (RID)	: 33

### 14.7. Maritime transport in bulk according to IMO instruments

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

##### REACH Annex XVII (Restriction List)

Not listed on REACH Annex XVII

##### REACH Annex XIV (Authorisation List)

Not listed on REACH Annex XIV (Authorisation List)

##### REACH Candidate List (SVHC)

Not listed on the REACH Candidate List

##### PIC Regulation (Prior Informed Consent)

Not listed on the PIC list (Regulation EU 649/2012)

##### POP Regulation (Persistent Organic Pollutants)

Not listed on the POP list (Regulation EU 2019/1021)

##### Ozone Regulation (1005/2009)

Not listed on the Ozone Depletion list (Regulation EU 1005/2009)

##### Dual-Use Regulation (428/2009)

Contains no substance subject to the COUNCIL REGULATION (EC) No 428/2009 of 5 May 2009 setting up a Community regime for the control of exports, transfer, brokering and transit of dual-use items.

##### Explosives Precursors Regulation (2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors)

##### Drug Precursors Regulation (273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

#### 15.1.2. National regulations

##### France

### Occupational diseases

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Code	Description
RG 84	Conditions caused by liquid organic solvents for professional use: saturated or unsaturated aliphatic or cyclic liquid hydrocarbons and mixtures thereof; liquid halogenated hydrocarbons; nitrated derivatives of aliphatic hydrocarbons; alcohols; glycols, glycol ethers; ketones; aldehydes; aliphatic and cyclic ethers, including tetrahydrofuran; esters; dimethylformamide and dimethylacetamine; acetonitrile and propionitrile; pyridine; dimethylsulfone and dimethylsulfoxide

### Germany

Water hazard class (WGK) : WGK 2, Significantly hazardous to water (Classification according to AwSV; ID No. 479).  
Hazardous Incident Ordinance (12. BImSchV) : Is not subject to the Hazardous Incident Ordinance (12. BImSchV)

### Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed  
SZW-lijst van mutagene stoffen : The substance is not listed  
SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed  
SZW-lijst van reprotoxische stoffen – Vruchtbaarheid : The substance is not listed  
SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

### Denmark

Classification remarks : Emergency management guidelines for the storage of flammable liquids must be followed  
Danish National Regulations : Young people below the age of 18 years are not allowed to use the product

## 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

## SECTION 16: Other information

### Abbreviations and acronyms:

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
BLV	Biological limit value
BOD	Biochemical oxygen demand (BOD)
COD	Chemical oxygen demand (COD)
DMEL	Derived Minimal Effect level
DNEL	Derived-No Effect Level
EC-No.	European Community number
EC50	Median effective concentration
EN	European Standard
IARC	International Agency for Research on Cancer
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
LOAEL	Lowest Observed Adverse Effect Level
NOAEC	No-Observed Adverse Effect Concentration
NOAEL	No-Observed Adverse Effect Level

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### Abbreviations and acronyms:

NOEC	No-Observed Effect Concentration
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
PBT	Persistent Bioaccumulative Toxic
PNEC	Predicted No-Effect Concentration
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
STP	Sewage treatment plant
ThOD	Theoretical oxygen demand (ThOD)
TLM	Median Tolerance Limit
VOC	Volatile Organic Compounds
CAS-No.	Chemical Abstract Service number
N.O.S.	Not Otherwise Specified
vPvB	Very Persistent and Very Bioaccumulative
ED	Endocrine disrupting properties

### Full text of H- and EUH-statements:

Aquatic Acute 1	Hazardous to the aquatic environment – Acute Hazard, Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment – Chronic Hazard, Category 1
Asp. Tox. 1	Aspiration hazard, Category 1
Flam. Liq. 2	Flammable liquids, Category 2
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity – Single exposure, Category 3, Narcosis

Safety Data Sheet (SDS), EU

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.