

n-OCTANE FOR SYNTHESIS

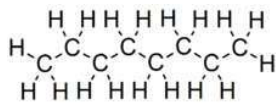
Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878
Reference number: 5037K
Issue date: 1/29/2024 Revision date: 1/29/2026 Supersedes version of: 7/27/2013 Version: 1.0



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

1.1. Product identifier

Product form	: Substance
Trade name	: n-OCTANE FOR SYNTHESIS
EC Index-No.	: 601-009-00-8
EC-No.	: 203-892-1
CAS-No.	: 111-65-9
Product code	: B-01880
Type of product	: Hydrocarbons, aliphatic
Formula	: C ₈ H ₁₈
Chemical structure	: 
Synonyms	: Octane, Octacarbane

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

1.2.1. Relevant identified uses

Use of the substance/mixture	: Laboratory chemicals, Manufacture of substances
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1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Bio-Chem Chemicals
5455, Nicholson Road Science Market,
Ambala Cantt. 133001 Haryana (India)
+91-82952 41953
info@biofinechemical.com - www.biofinechemical.com

1.4. Emergency telephone number

Emergency number	: +91 99921 51495 (10.00am - 06.30pm) (Office Hours)
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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,	H336
Narcosis	
Aspiration hazard, Category 1	H304
Hazardous to the aquatic environment – Acute Hazard,	H400
Category 1	
Hazardous to the aquatic environment – Chronic Hazard,	H410
Category 1	

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.

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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.
P233 - Keep container tightly closed.
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 .
P331 - Do NOT induce vomiting.

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	%
n-OCTANE	CAS-No.: 111-65-9 EC-No.: 203-892-1 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

First-aid measures after ingestion

- : 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.
- : Rinse skin with water/shower. Take off immediately all contaminated clothing. Wash with plenty of water/.... Wash contaminated clothing before reuse. If skin irritation occurs: Get medical advice/attention. Specific treatment (see supplemental first aid instruction on this label). If skin irritation occurs: Get medical advice/attention.
- : Remove contact lenses, if present and easy to do. Continue rinsing. Rinse cautiously with water for several minutes. If eye irritation persists: Get medical advice/attention.
- : Immediately call a POISON CENTER/doctor. Do not induce vomiting. Call a physician immediately.

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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	: dry chemical powder, alcohol-resistant foam, carbon dioxide (CO ₂). Water spray. Dry powder. Foam. Carbon dioxide.
Unsuitable extinguishing media	: Do not use a heavy water stream.

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 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.
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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. Avoid breathing dust/fume/gas/mist/vapours/spray. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures	: Stop release. Evacuate unnecessary personnel. Stop leak if safe to do so.

6.2. Environmental precautions

Avoid release to the environment.

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.
Methods for cleaning up	: Take up liquid spill into absorbent material. Collect spillage. On land, sweep or shovel into suitable containers. Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible. Notify authorities if product enters sewers or public waters.
Other information	: Dispose of materials or solid residues at an authorized site.

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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

: No open flames. No smoking. Use only non-sparking tools. Avoid breathing dust/fume/gas/mist/vapours/spray. Use only outdoors or in a well-ventilated area. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Take precautionary measures against static discharge. Flammable vapours may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Avoid contact with skin and eyes.

Hygiene measures

: Wash hands, forearms and face thoroughly after handling. 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. Use explosion-proof electrical/ventilating/lighting equipment.

Storage conditions

: Keep in fireproof place. Keep container tightly closed. Store in a well-ventilated place. Keep cool. 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.

8.2.2. Personal protection equipment

Personal protective equipment:

Wear recommended personal protective equipment.

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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	: gasoline-like.
Odour threshold	: Not available
Melting point	: Not applicable
Freezing point	: -57.1 – -56.6 °C
Boiling point	: 125 – 127 °C
Flammability	: Highly flammable liquid and vapour.
Lower explosion limit	: 0.96 vol %
Upper explosion limit	: 6.5 vol %
Flash point	: 13 °C
Auto-ignition temperature	: 220 °C
Decomposition temperature	: Not available
pH	: Not available
Viscosity, kinematic	: 0.733 mm ² /s
Viscosity, dynamic	: 0.515 cP at 25 °C
Solubility	: Water: Immiscible Ethanol: Miscible
Partition coefficient n-octanol/water (Log Kow)	: Not available
Vapour pressure	: 14.1 mm Hg at 25 °C
Vapour pressure at 50°C	: Not available
Density	: 0.703 g/cm ³ at 20 °C
Relative density	: Not available
Relative vapour density at 20°C	: 3.86 (Air= 1)
Particle characteristics	: Not applicable

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9.2. Other information

9.2.1. Information with regard to physical hazard classes

No additional information available

9.2.2. Other safety characteristics

Relative evaporation rate (butylacetate=1) : 0.6

SECTION 10: Stability and reactivity

10.1. Reactivity

Highly flammable liquid and vapour.

10.2. Chemical stability

Highly 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

Open flame. Direct sunlight. 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	0.733 mm ² /s
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11.2. Information on other hazards

No additional information available

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Very toxic to aquatic life with long lasting effects.

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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

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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

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

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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
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

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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

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

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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)

EU restriction list (REACH Annex XVII)	
Reference code	Applicable on
3(a)	n-OCTANE FOR SYNTHESIS
3(b)	n-OCTANE FOR SYNTHESIS
3(c)	n-OCTANE FOR SYNTHESIS
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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)

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15.1.2. National regulations

France

Occupational diseases	
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 of 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

Class for fire hazard : Class I-1
Store unit : 1 liter
Classification remarks : F <Flam. Liq. 2>; 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

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Abbreviations and acronyms:	
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
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.