

MB031 - DTT

Date of compilation: 06/01/2020

Version: 1

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifier: MB031 - DTT

(R*,R*)-1,4-dimercaptobutane-2,3-diol

CAS: 3483-12-3

EC: 222-468-7

Index: Non-applicable

REACH: Non-applicable

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

Relevant uses: Laboratory. For professional user only.

Uses advised against: All uses not specified in this section or in section 7.3

1.3 Details of the supplier of the safety data sheet:

NZYTech

Estrada do Paco do Lumiar Campus do Lumiar - Edif. E, r/c

1649-038 Lisboa - Lisboa - Portugal

info@nzytech.com

www.nzytech.com

1.4 Emergency telephone number: +351 213 643 514

Local time: Monday to Friday 9.00 am to 18.00

National Poison Information Centre (Europe UK): +44 0845 4647 (this service is only available to health professionals)

SECTION 2: HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture:

CLP Regulation (EC) No 1272/2008:

Classification of this product has been carried out in accordance with CLP Regulation (EC) No 1272/2008.

Acute Tox. 4: Acute toxicity if swallowed, Category 4, H302

Eye Irrit. 2: Eye irritation, Category 2, H319

Skin Irrit. 2: Skin irritation, Category 2, H315

STOT SE 3: Respiratory tract toxicity, single exposure, Category 3, H335

2.2 Label elements:

CLP Regulation (EC) No 1272/2008:

Warning



Hazard statements:

Acute Tox. 4: H302 - Harmful if swallowed

Eye Irrit. 2: H319 - Causes serious eye irritation

Skin Irrit. 2: H315 - Causes skin irritation

STOT SE 3: H335 - May cause respiratory irritation

Precautionary statements:

P264: Wash thoroughly after handling

P271: Use only outdoors or in a well-ventilated area

P280: Wear protective gloves/protective clothing/eye protection/face protection

P302+P352: IF ON SKIN: Wash with plenty of water

P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing

P305+P351+P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P403+P233: Store in a well-ventilated place. Keep container tightly closed

P501: Dispose of contents/container in accordance with regulations on hazardous waste or packaging and packaging waste respectively

2.3 Other hazards:

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SECTION 2: HAZARDS IDENTIFICATION (continued)

Product fails to meet PBT/vPvB criteria

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substance:

Chemical description: Organic substance

Components:

In accordance with Annex II of Regulation (EC) No 1907/2006 (point 3), the product contains:

| Identification | Chemical name/Classification | Concentration |
|---|--|---------------------------------|
| CAS: 3483-12-3 EC: 222-468-7 Index: Non-applicable REACH: Non-applicable | (R*,R*)-1,4-dimercaptobutane-2,3-diol Regulation 1272/2008 Acute Tox. 4: H302; Eye Irrit. 2: H319; Skin Irrit. 2: H315; STOT SE 3: H335 - Warning | Self-classified 100 % |

To obtain more information on the hazards of the substances consult sections 11, 12 and 16.

3.2 Mixture:

Non-applicable

SECTION 4: FIRST AID MEASURES

4.1 Description of first aid measures:

The symptoms resulting from intoxication can appear after exposure, therefore, in case of doubt, seek medical attention for direct exposure to the chemical product or persistent discomfort, showing the SDS of this product.

By inhalation:

Remove the person affected from the area of exposure, provide with fresh air and keep at rest. In serious cases such as cardiorespiratory failure, artificial resuscitation techniques will be necessary (mouth to mouth resuscitation, cardiac massage, oxygen supply, etc.) requiring immediate medical assistance.

By skin contact:

Remove contaminated clothing and footwear, rinse skin or shower the person affected if appropriate with plenty of cold water and neutral soap. In serious cases see a doctor. If the product causes burns or freezing, clothing should not be removed as this could worsen the injury caused if it is stuck to the skin. If blisters form on the skin, these should never be burst as this will increase the risk of infection.

By eye contact:

Rinse eyes thoroughly with lukewarm water for at least 15 minutes. Do not allow the person affected to rub or close their eyes. If the injured person uses contact lenses, these should be removed unless they are stuck to the eyes, in which case this could cause further damage. In all cases, after cleaning, a doctor should be consulted as quickly as possible with the SDS of the product.

By ingestion/aspiration:

Request medical assistance immediately, showing the SDS of this product. Do not induce vomiting, but if it does happen keep the head down to avoid aspiration. In the case of loss of consciousness do not administer anything orally unless supervised by a doctor. Rinse out the mouth and throat, as they may have been affected during ingestion. Keep the person affected at rest.

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

Acute and delayed effects are indicated in sections 2 and 11.

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

Non-applicable

SECTION 5: FIREFIGHTING MEASURES

5.1 Extinguishing media:

Product is non-flammable under normal conditions of storage, handling and use. In the case of combustion as a result of improper handling, storage or use preferably use polyvalent powder extinguishers (ABC powder), in accordance with the Regulation on fire protection systems. IT IS NOT RECOMMENDED to use full jet water as an extinguishing agent.

5.2 Special hazards arising from the substance or mixture:

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SECTION 5: FIREFIGHTING MEASURES (continued)

As a result of combustion or thermal decomposition reactive sub-products are created that can become highly toxic and, consequently, can present a serious health risk.

5.3 Advice for firefighters:

Depending on the magnitude of the fire it may be necessary to use full protective clothing and self-contained breathing apparatus (SCBA). Minimum emergency facilities and equipment should be available (fire blankets, portable first aid kit,...) in accordance with Directive 89/654/EC.

Additional provisions:

Act in accordance with the Internal Emergency Plan and the Information Sheets on actions to take after an accident or other emergencies. Eliminate all sources of ignition. In case of fire, cool the storage containers and tanks for products susceptible to combustion, explosion or BLEVE as a result of high temperatures. Avoid spillage of the products used to extinguish the fire into an aqueous medium.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures:

Sweep up and shovel product or collect by other means and place in container for reuse (preferred) or disposal

6.2 Environmental precautions:

This product is not classified as hazardous to the environment. Keep product away from drains, surface and ground water.

6.3 Methods and material for containment and cleaning up:

It is recommended:

Sweep up and shovel product or collect by other means and place in container for reuse (preferred) or disposal

6.4 Reference to other sections:

See sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1 Precautions for safe handling:

A.- Precautions for safe manipulation

Comply with the current legislation concerning the prevention of industrial risks. Keep containers hermetically sealed. Control spills and residues, destroying them with safe methods (section 6). Avoid leakages from the container. Maintain order and cleanliness where dangerous products are used.

B.- Technical recommendations for the prevention of fires and explosions

Due to its non-flammable nature, the product does not present a fire risk under normal conditions of storage, handling and use.

C.- Technical recommendations to prevent ergonomic and toxicological risks

Do not eat or drink during the process, washing hands afterwards with suitable cleaning products.

D.- Technical recommendations to prevent environmental risks

It is recommended to have absorbent material available at close proximity to the product (See subsection 6.3)

7.2 Conditions for safe storage, including any incompatibilities:

A.- Technical measures for storage

Store in a cool, dry, well-ventilated location

B.- General conditions for storage

Avoid sources of heat, radiation, static electricity and contact with food. For additional information see subsection 10.5

7.3 Specific end use(s):

Except for the instructions already specified it is not necessary to provide any special recommendation regarding the uses of this product.

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters:

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SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION (continued)

Substances whose occupational exposure limits have to be monitored in the workplace

Nuisance dust: Inhalable dust 10 mg/m³ // Respirable dust 4 mg/m³

DNEL (Workers):

Non-applicable

DNEL (General population):

Non-applicable

PNEC:

Non-applicable



8.2 Exposure controls:

A.- General security and hygiene measures in the work place



As a preventative measure it is recommended to use basic Personal Protective Equipment, with the corresponding <<CE marking>> in accordance with Directive 89/686/EC. For more information on Personal Protective Equipment (storage, use, cleaning, maintenance, class of protection,...) consult the information leaflet provided by the manufacturer. For more information see subsection 7.1.

All information contained herein is a recommendation which needs some specification from the labour risk prevention services as it is not known whether the company has additional measures at its disposal.



B.- Respiratory protection

| Pictogram | PPE | Labelling | CEN Standard | Remarks |
|--|-----------------------------------|---|---------------------|--|
|  Mandatory respiratory tract protection | Filter mask for gases and vapours |  CAT III | EN 405:2001+A1:2009 | Replace when there is a taste or smell of the contaminant inside the face mask. If the contaminant comes with warnings it is recommended to use isolation equipment. |



C.- Specific protection for the hands

| Pictogram | PPE | Labelling | CEN Standard | Remarks |
|--|---------------------------------------|--|--------------|--|
|  Mandatory hand protection | Protective gloves against minor risks |  CAT I | | Replace gloves in case of any sign of damage. For prolonged periods of exposure to the product for professional users/industrials, we recommend using CE III gloves in line with standards EN 420:2003+A1:2009 and EN ISO 374-1:2016 |

D.- Ocular and facial protection

| Pictogram | PPE | Labelling | CEN Standard | Remarks |
|--|---|---|---------------------------------|---|
|  Mandatory face protection | Panoramic glasses against splash/projections. |  CAT II | EN 166:2001 EN ISO 4007:2018 | Clean daily and disinfect periodically according to the manufacturer's instructions. Use if there is a risk of splashing. |



E.- Body protection

| Pictogram | PPE | Labelling | CEN Standard | Remarks |
|-----------|----------------------|---|-------------------|---|
| | Work clothing |  CAT I | | Replace before any evidence of deterioration. For periods of prolonged exposure to the product for professional/industrial users CE III is recommended, in accordance with the regulations in EN ISO 6529:2013, EN ISO 6530:2005, EN ISO 13688:2013, EN 464:1994. |
| | Anti-slip work shoes |  CAT II | EN ISO 20347:2012 | Replace before any evidence of deterioration. For periods of prolonged exposure to the product for professional/industrial users CE III is recommended, in accordance with the regulations in EN ISO 20345:2012 y EN 13832-1:2007 |

F.- Additional emergency measures

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SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION (continued)

| Emergency measure | Standards | Emergency measure | Standards |
|---|---|--|--|
|  Emergency shower | ANSI Z358-1 ISO 3864-1:2011, ISO 3864-4:2011 |  Eyewash stations | DIN 12 899 ISO 3864-1:2011, ISO 3864-4:2011 |

Environmental exposure controls:

In accordance with the community legislation for the protection of the environment it is recommended to avoid environmental spillage of both the product and its container. For additional information see subsection 7.1.D

Volatile organic compounds:

With regard to Directive 2010/75/EU, this product has the following characteristics:

| | |
|---------------------------|-----------------------------|
| V.O.C. (Supply): | 0 % weight |
| V.O.C. density at 20 °C: | 0 kg/m ³ (0 g/L) |
| Average carbon number: | Non-applicable |
| Average molecular weight: | Non-applicable |

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties:

For complete information see the product datasheet.

Appearance:

| | |
|--------------------------|------------------|
| Physical state at 20 °C: | Solid |
| Appearance: | Not available |
| Colour: | White |
| Odour: | Not available |
| Odour threshold: | Non-applicable * |

Volatility:

| | |
|--|------------------|
| Boiling point at atmospheric pressure: | Non-applicable * |
| Vapour pressure at 20 °C: | Non-applicable * |
| Vapour pressure at 50 °C: | Non-applicable * |
| Evaporation rate at 20 °C: | Non-applicable * |

Product description:

| | |
|--|------------------------|
| Density at 20 °C: | 1300 kg/m ³ |
| Relative density at 20 °C: | 1,3 |
| Dynamic viscosity at 20 °C: | Non-applicable * |
| Kinematic viscosity at 20 °C: | Non-applicable * |
| Kinematic viscosity at 40 °C: | Non-applicable * |
| Concentration: | Non-applicable * |
| pH: | 4 - 6 |
| Vapour density at 20 °C: | Non-applicable * |
| Partition coefficient n-octanol/water 20 °C: | Non-applicable * |
| Solubility in water at 20 °C: | 15,4 kg/m ³ |
| Solubility properties: | Non-applicable * |
| Decomposition temperature: | Non-applicable * |
| Melting point/freezing point: | 40 - 44 °C |
| Explosive properties: | Non-applicable * |
| Oxidising properties: | Non-applicable * |

*Not relevant due to the nature of the product, not providing information property of its hazards.

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SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES (continued)

Flammability:

| | |
|----------------------------|------------------|
| Flash Point: | 113 °C |
| Flammability (solid, gas): | Non-applicable * |
| Autoignition temperature: | Non-applicable * |
| Lower flammability limit: | Non-applicable * |
| Upper flammability limit: | Non-applicable * |

Explosive:

| | |
|------------------------|------------------|
| Lower explosive limit: | Non-applicable * |
| Upper explosive limit: | Non-applicable * |

9.2 Other information:

| | |
|---------------------------|------------------|
| Surface tension at 20 °C: | Non-applicable * |
| Refraction index: | Non-applicable * |

*Not relevant due to the nature of the product, not providing information property of its hazards.

SECTION 10: STABILITY AND REACTIVITY

10.1 Reactivity:

No hazardous reactions are expected because the product is stable under recommended storage conditions. See section 7.

10.2 Chemical stability:

Chemically stable under the conditions of storage, handling and use.

10.3 Possibility of hazardous reactions:

Under the specified conditions, hazardous reactions that lead to excessive temperatures or pressure are not expected.

10.4 Conditions to avoid:

Applicable for handling and storage at room temperature:

| Shock and friction | Contact with air | Increase in temperature | Sunlight | Humidity |
|--------------------|------------------|-------------------------|----------------|----------------|
| Not applicable | Not applicable | Not applicable | Not applicable | Not applicable |

10.5 Incompatible materials:

| Acids | Water | Oxidising materials | Combustible materials | Others |
|--------------------|----------------|---------------------|-----------------------|-------------------------------|
| Avoid strong acids | Not applicable | Not applicable | Not applicable | Avoid alkalis or strong bases |

10.6 Hazardous decomposition products:

See subsection 10.3, 10.4 and 10.5 to find out the specific decomposition products. Depending on the decomposition conditions, complex mixtures of chemical substances can be released: carbon dioxide (CO₂), carbon monoxide and other organic compounds.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects:

The experimental information related to the toxicological properties of the product itself is not available

Dangerous health implications:

In case of exposure that is repetitive, prolonged or at concentrations higher than the recommended occupational exposure limits, adverse effects on health may result, depending on the means of exposure:

A- Ingestion (acute effect):

- Acute toxicity : The consumption of a considerable dose can cause irritation in the throat, abdominal pain, nausea and vomiting.
- Corrosivity/Irritability: The consumption of a considerable dose can cause irritation in the throat, abdominal pain, nausea and vomiting.

B- Inhalation (acute effect):

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SECTION 11: TOXICOLOGICAL INFORMATION (continued)

- Acute toxicity : Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for inhalation. For more information see section 3.
- Corrosivity/Irritability: Causes irritation in respiratory passages, which is normally reversible and limited to the upper respiratory passages.
- C- Contact with the skin and the eyes (acute effect):
 - Contact with the skin: Produces skin inflammation.
 - Contact with the eyes: Produces eye damage after contact.
- D- CMR effects (carcinogenicity, mutagenicity and toxicity to reproduction):
 - Carcinogenicity: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for the effects mentioned. For more information see section 3.
IARC: Non-applicable
 - Mutagenicity: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.
 - Reproductive toxicity: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.
- E- Sensitizing effects:
 - Respiratory: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous with sensitising effects. For more information see section 3.
 - Cutaneous: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.
- F- Specific target organ toxicity (STOT) - single exposure:

Causes irritation in respiratory passages, which is normally reversible and limited to the upper respiratory passages.
- G- Specific target organ toxicity (STOT)-repeated exposure:
 - Specific target organ toxicity (STOT)-repeated exposure: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.
 - Skin: Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.
- H- Aspiration hazard:

Based on available data, the classification criteria are not met, as it does not contain substances classified as dangerous for this effect. For more information see section 3.

Other information:

Non-applicable

Specific toxicology information on the substances:

| Identification | Acute toxicity | | Genus |
|---------------------------------------|-----------------|---------------|-------|
| (R*,R*)-1,4-dimercaptobutane-2,3-diol | LD50 oral | 400 mg/kg | Rat |
| CAS: 3483-12-3 | LD50 dermal | >2000 mg/kg | |
| EC: 222-468-7 | LC50 inhalation | >5 mg/L (4 h) | |

SECTION 12: ECOLOGICAL INFORMATION

12.1 Toxicity:

Not available

12.2 Persistence and degradability:

Not available

12.3 Bioaccumulative potential:

Not available

12.4 Mobility in soil:

Not available

12.5 Results of PBT and vPvB assessment:

Product fails to meet PBT/vPvB criteria

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SECTION 12: ECOLOGICAL INFORMATION (continued)

12.6 Other adverse effects:

Not described

SECTION 13: DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods:

| Code | Description | Waste class (Regulation (EU) No 1357/2014) |
|-----------|--|--|
| 16 03 05* | organic wastes containing hazardous substances | Dangerous |

Type of waste (Regulation (EU) No 1357/2014):

HP5 Specific Target Organ Toxicity (STOT)/Aspiration Toxicity, HP6 Acute Toxicity, HP4 Irritant — skin irritation and eye damage

Waste management (disposal and evaluation):

Consult the authorized waste service manager on the assessment and disposal operations in accordance with Annex 1 and Annex 2 (Directive 2008/98/EC). As under 15 01 (2014/955/EC) of the code and in case the container has been in direct contact with the product, it will be processed the same way as the actual product. Otherwise, it will be processed as non-dangerous residue. We do not recommend disposal down the drain. See paragraph 6.2.

Regulations related to waste management:

In accordance with Annex II of Regulation (EC) No 1907/2006 (REACH) the community or state provisions related to waste management are stated

Community legislation: Directive 2008/98/EC, 2014/955/EU, Regulation (EU) No 1357/2014

SECTION 14: TRANSPORT INFORMATION

Transport of dangerous goods by land:

With regard to ADR 2019 and RID 2019:

- | | |
|---|----------------|
| 14.1 UN number: | Non-applicable |
| 14.2 UN proper shipping name: | Non-applicable |
| 14.3 Transport hazard class(es): | Non-applicable |
| Labels: | Non-applicable |
| 14.4 Packing group: | Non-applicable |
| 14.5 Environmental hazards: | No |
| 14.6 Special precautions for user | |
| Special regulations: | Non-applicable |
| Tunnel restriction code: | Non-applicable |
| Physico-Chemical properties: | see section 9 |
| Limited quantities: | Non-applicable |
| 14.7 Transport in bulk according to Annex II of Marpol and the IBC Code: | Non-applicable |

Transport of dangerous goods by sea:

With regard to IMDG 38-16:

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SECTION 14: TRANSPORT INFORMATION (continued)

| | |
|---|----------------|
| 14.1 UN number: | Non-applicable |
| 14.2 UN proper shipping name: | Non-applicable |
| 14.3 Transport hazard class(es): | Non-applicable |
| Labels: | Non-applicable |
| 14.4 Packing group: | Non-applicable |
| 14.5 Environmental hazards: | No |
| 14.6 Special precautions for user | |
| Special regulations: | Non-applicable |
| EmS Codes: | |
| Physico-Chemical properties: | see section 9 |
| Limited quantities: | Non-applicable |
| Segregation group: | Non-applicable |
| 14.7 Transport in bulk according to Annex II of Marpol and the IBC Code: | Non-applicable |

Transport of dangerous goods by air:

With regard to IATA/ICAO 2019:

| | |
|---|----------------|
| 14.1 UN number: | Non-applicable |
| 14.2 UN proper shipping name: | Non-applicable |
| 14.3 Transport hazard class(es): | Non-applicable |
| Labels: | Non-applicable |
| 14.4 Packing group: | Non-applicable |
| 14.5 Environmental hazards: | No |
| 14.6 Special precautions for user | |
| Physico-Chemical properties: | see section 9 |
| 14.7 Transport in bulk according to Annex II of Marpol and the IBC Code: | Non-applicable |

SECTION 15: REGULATORY INFORMATION

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

Candidate substances for authorisation under the Regulation (EC) No 1907/2006 (REACH): Non-applicable

Substances included in Annex XIV of REACH ("Authorisation List") and sunset date: Non-applicable

Regulation (EC) No 1005/2009, about substances that deplete the ozone layer: Non-applicable

Article 95, REGULATION (EU) No 528/2012: Non-applicable

REGULATION (EU) No 649/2012, in relation to the import and export of hazardous chemical products: Non-applicable

Seveso III:

Non-applicable

Limitations to commercialisation and the use of certain dangerous substances and mixtures (Annex XVII REACH, etc):

Non-applicable

Specific provisions in terms of protecting people or the environment:

It is recommended to use the information included in this safety data sheet as a basis for conducting workplace-specific risk assessments in order to establish the necessary risk prevention measures for the handling, use, storage and disposal of this product.

Other legislation:

The product could be affected by sectorial legislation

15.2 Chemical safety assessment:

The supplier has not carried out evaluation of chemical safety.

SECTION 16: OTHER INFORMATION**Legislation related to safety data sheets:**

This safety data sheet has been designed in accordance with ANNEX II-Guide to the compilation of safety data sheets of Regulation (EC) No 1907/2006 (Regulation (EC) No 2015/830)

Modifications related to the previous Safety Data Sheet which concerns the ways of managing risks.:

Non-applicable

Texts of the legislative phrases mentioned in section 2:

H302: Harmful if swallowed

H315: Causes skin irritation

H335: May cause respiratory irritation

H319: Causes serious eye irritation

Texts of the legislative phrases mentioned in section 3:

The phrases indicated do not refer to the product itself; they are present merely for informative purposes and refer to the individual components which appear in section 3

CLP Regulation (EC) No 1272/2008:

Acute Tox. 4: H302 - Harmful if swallowed

Eye Irrit. 2: H319 - Causes serious eye irritation

Skin Irrit. 2: H315 - Causes skin irritation

STOT SE 3: H335 - May cause respiratory irritation

Advice related to training:

Minimal training is recommended in order to prevent industrial risks for staff using this product and to facilitate their comprehension and interpretation of this safety data sheet, as well as the label on the product.

Principal bibliographical sources:

<http://echa.europa.eu>

<http://eur-lex.europa.eu>

Abbreviations and acronyms:

ADR: European agreement concerning the international carriage of dangerous goods by road

IMDG: International maritime dangerous goods code

IATA: International Air Transport Association

ICAO: International Civil Aviation Organisation

COD: Chemical Oxygen Demand

BOD5: 5-day biochemical oxygen demand

BCF: Bioconcentration factor

LD50: Lethal Dose 50

LC50: Lethal Concentration 50

EC50: Effective concentration 50

Log-POW: Octanol-water partition coefficient

Koc: Partition coefficient of organic carbon