

# SAFETY DATA SHEET

## TBPIN



Version 2.0      Revision Date: 19.11.2020      SDS Number: 600000000003      Date of last issue: 29.08.2019  
Date of first issue: 29.08.2019

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### SECTION 1: Identification of the hazardous chemical and of the supplier

#### Product identifier

Product name : TBPIN  
Chemical name : tert-butyl 3,5,5-trimethylperoxyhexanoate  
CAS-No. : 13122-18-4

#### Recommended use of the chemical and restrictions on use

Recommended use : polymerisation initiators

#### Manufacturer or supplier's details

Company : United Initiators GmbH  
Address : Dr.-Gustav-Adolph-Str. 3  
82049 Pullach  
Telephone : +49 / 89 / 74422 – 0  
Emergency telephone number : +49 / 89 / 74422 – 0 (24 h)  
E-mail address : contact@united-in.com

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### SECTION 2: Hazards identification

#### Classification of the hazardous chemical

Organic peroxides : Type D  
Skin sensitisation : Category 1  
Hazardous to the aquatic environment - acute hazard : Category 1  
Hazardous to the aquatic environment - chronic hazard : Category 1

#### Label elements

Hazard pictograms :

Signal word : Danger

Hazard statements : H242 Heating may cause a fire.  
H317 May cause an allergic skin reaction.

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H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements :

**Prevention:**

P210 Keep away from heat/sparks/open flames/hot surfaces.  
No smoking.

P220 Keep/Store away from clothing/ strong acids, bases,  
heavy metal salts and other reducing substances /combustible  
materials.

P234 Keep only in original container.

P273 Avoid release to the environment.

P280 Wear protective gloves/ eye protection/ face protection.

**Response:**

P391 Collect spillage.

**Storage:**

P411 + P235 Store at temperatures not exceeding < 30 °C/ <  
86 °F. Keep cool.

**Other hazards which do not result in classification**

None known.

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### SECTION 3: Composition and information of the ingredients of the hazardous chemical

Substance / Mixture : Substance

Chemical nature : Organic Peroxide  
liquid

**Components**

Chemical name	CAS-No.	Concentration (% w/w)
tert-butyl 3,5,5-trimethylperoxyhexanoate	13122-18-4	<= 100

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### SECTION 4: First aid measures

General advice : Move out of dangerous area.  
Show this safety data sheet to the doctor in attendance.  
Do not leave the victim unattended.  
Call a physician immediately.

If inhaled : If unconscious, place in recovery position and seek medical  
advice.  
If symptoms persist, call a physician.  
If breathed in, move person into fresh air.

In case of skin contact : In case of contact, immediately flush skin with plenty of water  
for at least 15 minutes while removing contaminated clothing  
and shoes.  
Wash contaminated clothing before re-use.  
If on skin, rinse well with water.  
If on clothes, remove clothes.

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- If symptoms persist, call a physician.
- In case of eye contact : In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.  
Remove contact lenses.  
Protect unharmed eye.  
Keep eye wide open while rinsing.  
If eye irritation persists, consult a specialist.
- If swallowed : Keep respiratory tract clear.  
Call a physician immediately.
- Most important symptoms and effects, both acute and delayed : May cause an allergic skin reaction.
- Protection of first-aiders : First Aid responders should pay attention to self-protection and use the recommended protective clothing
- Notes to physician : Treat symptomatically and supportively.
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### SECTION 5: Firefighting measures

#### Extinguishing media

Suitable extinguishing media : Water spray jet  
Alcohol-resistant foam  
Carbon dioxide (CO<sub>2</sub>)  
Dry chemical

Unsuitable extinguishing media : High volume water jet

#### Physicochemical hazards arising from the chemical

Specific hazards during fire-fighting : Contact with incompatible materials or exposure to temperatures exceeding SADT may result in a self-accelerating decomposition reaction with release of flammable vapors which may auto-ignite.  
The product burns violently.  
Flash back possible over considerable distance.  
Vapours may form explosive mixtures with air.  
The product will float on water and can be reignited on surface water.  
Cool closed containers exposed to fire with water spray.

#### Special protective equipment and precautions for fire-fighters

Special protective equipment for firefighters : Wear self-contained breathing apparatus for firefighting if necessary.  
Use personal protective equipment.

Specific extinguishing methods : Collect contaminated fire extinguishing water separately. This must not be discharged into drains.

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Fire residues and contaminated fire extinguishing water must be disposed of in accordance with local regulations. Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Do not use a solid water stream as it may scatter and spread fire.  
Remove undamaged containers from fire area if it is safe to do so.  
Use water spray to cool unopened containers.

Hazchem Code : 2WE

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### SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures : Use personal protective equipment.  
Remove all sources of ignition.  
Follow safe handling advice and personal protective equipment recommendations.  
Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.  
Never return spills in original containers for re-use.  
Treat recovered material as described in the section "Disposal considerations".

Environmental precautions : Prevent product from entering drains.  
Prevent further leakage or spillage if safe to do so.  
If the product contaminates rivers and lakes or drains inform respective authorities.

Methods and materials for containment and cleaning up : Contact with incompatible substances can cause decomposition at or below SADT.  
Clear spills immediately.  
Suppress (knock down) gases/vapours/mists with a water spray jet.  
To clean the floor and all objects contaminated by this material, use plenty of water.  
Soak up with inert absorbent material.  
Isolate waste and do not reuse.  
Non-sparking tools should be used.  
Local or national regulations may apply to releases and disposal of this material, as well as those materials and items employed in the cleanup of releases. You will need to determine which regulations are applicable.

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### SECTION 7: Handling and storage

#### Handling

#### Precautions for safe handling

Technical measures : See Engineering measures under EXPOSURE CONTROLS/PERSONAL PROTECTION section.

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- Advice on protection against fire and explosion : Keep away from heat and sources of ignition.  
Use only explosion-proof equipment.  
Keep away from combustible material.
- Advice on safe handling : Do not breathe vapours/dust.  
Avoid exposure - obtain special instructions before use.  
Avoid contact with skin and eyes.  
Avoid formation of aerosol.  
Take precautionary measures against static discharges.  
Never return any product to the container from which it was originally removed.  
Provide sufficient air exchange and/or exhaust in work rooms.  
Avoid confinement.  
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
Smoking, eating and drinking should be prohibited in the application area.  
Wash thoroughly after handling.  
For personal protection see section 8.  
Persons susceptible to skin sensitisation problems or asthma, allergies, chronic or recurrent respiratory disease should not be employed in any process in which this mixture is being used.  
Protect from contamination.

### Storage

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

- Conditions for safe storage : Avoid impurities (e.g. rust, dust, ash), risk of decomposition.  
Electrical installations / working materials must comply with the technological safety standards.  
Containers which are opened must be carefully resealed and kept upright to prevent leakage.  
Store in original container.  
Keep containers tightly closed in a cool, well-ventilated place.  
Store in accordance with the particular national regulations.
- Materials to avoid : Keep away from strong acids, bases, heavy metal salts and other reducing substances.
- Recommended storage temperature : < 30 °C
- Further information on storage stability : No decomposition if stored normally.

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## SECTION 8: Exposure controls and personal protection

### Control parameters

Contains no substances with occupational exposure limit values.

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**Appropriate engineering controls** : Minimize workplace exposure concentrations.

**Individual protection measures, such as personal protective equipment**

Eye/face protection : Tightly fitting safety goggles  
Please wear suitable protective goggles. Also wear face protection if there is a splash hazard.  
Ensure that eyewash stations and safety showers are close to the workstation location.

Skin protection : Select appropriate protective clothing based on chemical resistance data and an assessment of the local exposure potential.

Hand protection  
Material : butyl-rubber  
Break through time : 480 min  
Glove thickness : 0.5 mm

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.4 mm

Remarks : Choose gloves to protect hands against chemicals depending on the concentration and quantity of the hazardous substance and specific to place of work. For special applications, we recommend clarifying the resistance to chemicals of the aforementioned protective gloves with the glove manufacturer. Wash hands before breaks and at the end of workday.

Respiratory protection : In the case of dust or aerosol formation use respirator with an approved filter.

Filter type : ABEK-filter

Hygiene measures : Keep away from food and drink.  
When using do not eat or drink.  
When using do not smoke.  
Wash hands before breaks and immediately after handling the product.

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### SECTION 9: Physical and chemical properties

Appearance : liquid

Colour : colourless

Odour : very faint, ester-like

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Odour Threshold : No data available

pH : No data available

Melting point/freezing point : < -25 °C  
(1,013 hPa)

Initial boiling point and boiling range : Decomposition: Decomposes below the boiling point.

Flash point : 94 °C  
Method: ISO 3679

Evaporation rate : No data available

Flammability (solid, gas) : Not applicable

Upper explosion limit / Upper flammability limit : No data available

Lower explosion limit / Lower flammability limit : No data available

Vapour pressure : 0.03 hPa (30 °C)

Relative vapour density : No data available

Density : 0.89 g/cm<sup>3</sup> (20 °C)

Solubility(ies)  
Water solubility : 0.0142 g/l insoluble (20 °C)

Partition coefficient: n-octanol/water : log Pow: 5.16

Self-Accelerating decomposition temperature (SADT) : 60 °C  
Method: UN-Test H.4  
SADT-Self Accelerating Decomposition Temperature. Lowest temperature at which the tested package size will undergo a self-accelerating decomposition reaction.

Viscosity  
Viscosity, dynamic : 5 mPa.s (20 °C)

Explosive properties : Not explosive

Oxidizing properties : The substance or mixture is not classified as oxidizing.  
Organic peroxide

Refractive index : 1.431 (20 °C)

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### SECTION 10: Stability and reactivity

- Reactivity : Stable under recommended storage conditions.
- Chemical stability : Stable under recommended storage conditions.
- Possibility of hazardous reactions : Vapours may form explosive mixture with air.
- Conditions to avoid : Protect from contamination.  
Contact with incompatible substances can cause decomposition at or below SADT.  
Heat, flames and sparks.  
Avoid confinement.
- Incompatible materials : Accelerators, strong acids and bases, heavy metals and heavy metal salts, reducing agents
- Hazardous decomposition products : Irritant, caustic, flammable, noxious/toxic gases and vapours can develop in the case of fire and decomposition
- 

### SECTION 11: Toxicological information

Information on likely routes of exposure : None known.

#### Acute toxicity

Not classified based on available information.

#### Components:

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

- Acute oral toxicity : LD50 (Rat): 12,905 mg/kg  
Method: OECD Test Guideline 401
- Acute inhalation toxicity : LC50 (Rat): > 0.8 mg/l  
Exposure time: 4 h  
Test atmosphere: dust/mist  
Method: OECD Test Guideline 403  
Assessment: The substance or mixture has no acute inhalation toxicity
- Acute dermal toxicity : LD0 (Rat): > 2,000 mg/kg  
Method: OECD Test Guideline 402

#### **Skin corrosion/irritation**

Not classified based on available information.

#### Product:

- Remarks : May cause skin irritation in susceptible persons.



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### Components:

#### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Species : Rabbit  
Method : OECD Test Guideline 404  
Result : No skin irritation

#### **Serious eye damage/eye irritation**

Not classified based on available information.

### Product:

Remarks : Vapours may cause irritation to the eyes, respiratory system and the skin.

### Components:

#### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Species : Rabbit  
Result : No eye irritation  
Method : OECD Test Guideline 405

#### **Respiratory or skin sensitisation**

##### **Skin sensitisation**

May cause an allergic skin reaction.

##### **Respiratory sensitisation**

Not classified based on available information.

### Product:

Remarks : Causes sensitisation.

### Components:

#### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Exposure routes : Skin contact  
Species : Guinea pig  
Method : OECD Test Guideline 406  
Result : May cause sensitisation by skin contact.

#### **Germ cell mutagenicity**

Not classified based on available information.

### Components:

#### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Genotoxicity in vitro : Test Type: Bacterial reverse mutation assay (AMES)  
Method: OECD Test Guideline 471  
Result: negative

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Method: OECD Test Guideline 473  
Result: positive

Method: OECD Test Guideline 476  
Result: negative

Genotoxicity in vivo : Species: Rat  
Application Route: Oral  
Method: OECD Test Guideline 474  
Result: negative

### **Carcinogenicity**

Not classified based on available information.

#### **Components:**

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Remarks : This information is not available.

### **Reproductive toxicity**

Not classified based on available information.

#### **Components:**

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Effects on fertility : Test Type: Reproduction/Developmental toxicity screening test  
Species: Rat  
Application Route: Oral  
General Toxicity - Parent: NOAEL: 50 mg/kg body weight  
Method: OECD Test Guideline 421

Effects on foetal development : Test Type: Embryo-foetal development  
Species: Rat  
Application Route: Oral  
General Toxicity Maternal: NOAEL: 150 mg/kg body weight  
Method: OECD Test Guideline 414  
Result: negative

### **STOT - single exposure**

Not classified based on available information.

### **STOT - repeated exposure**

Not classified based on available information.

### **Repeated dose toxicity**

#### **Components:**

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Species : Rat, male and female  
NOAEL : 160 mg/kg  
Application Route : oral (gavage)

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Exposure time : 90 d  
Method : OECD Test Guideline 408

Species : Rat, male and female  
NOAEL : 50 mg/kg  
Application Route : oral (gavage)  
Exposure time : 28 d  
Method : OECD Test Guideline 407

### Aspiration toxicity

Not classified based on available information.

### Further information

#### Product:

Remarks : No data available

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## SECTION 12: Ecological information

### Ecotoxicity

#### Product:

#### Ecotoxicology Assessment

Acute aquatic toxicity : Very toxic to aquatic life.

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

#### Components:

#### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 7.03 mg/l  
Exposure time: 96 h  
Method: OECD Test Guideline 203

NOEC (Oncorhynchus mykiss (rainbow trout)): 3 mg/l  
Exposure time: 96 h  
Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): > 0.52 mg/l  
Exposure time: 48 h  
Method: OECD Test Guideline 202

Toxicity to algae/aquatic plants : NOEC (Pseudokirchneriella subcapitata (algae)): 0.04 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201

EC50 (Pseudokirchneriella subcapitata (algae)): 0.51 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201

M-Factor (Acute aquatic tox- : 1

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icity)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 0.22 mg/l  
Exposure time: 21 d  
Method: OECD Test Guideline 211

M-Factor (Chronic aquatic toxicity) : 1

Toxicity to microorganisms : EC50 (Bacteria): 327.02 mg/l  
Exposure time: 3 h  
Method: OECD Test Guideline 209

### Persistence and degradability

#### Components:

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Biodegradability : Result: Not readily biodegradable.  
Method: OECD Test Guideline 301D

### Bioaccumulative potential

#### Components:

##### **tert-butyl 3,5,5-trimethylperoxyhexanoate:**

Partition coefficient: n-octanol/water : log Pow: 5.16

### Mobility in soil

No data available

### Other adverse effects

#### Product:

Additional ecological information : An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Very toxic to aquatic life with long lasting effects.

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## SECTION 13: Disposal information

### Disposal methods

Waste from residues : The product should not be allowed to enter drains, water courses or the soil.  
Do not contaminate ponds, waterways or ditches with chemical or used container.  
Dispose of wastes in an approved waste disposal facility.

Contaminated packaging : Empty remaining contents.  
Dispose of as unused product.  
Do not re-use empty containers.

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Do not burn, or use a cutting torch on, the empty drum.  
Dispose of in accordance with local regulations.

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### SECTION 14: Transport information

#### International Regulations

##### UNRTDG

UN number : UN 3105  
Proper shipping name : ORGANIC PEROXIDE TYPE D, LIQUID  
(tert-BUTYL PEROXY-3,5,5-TRIMETHYLHEXANOATE)  
Class : 5.2  
Packing group : Not assigned by regulation  
Labels : 5.2

##### IATA-DGR

UN/ID No. : UN 3105  
Proper shipping name : Organic peroxide type D, liquid  
(tert-Butyl peroxy-3,5,5-trimethylhexanoate)  
Class : 5.2  
Packing group : Not assigned by regulation  
Labels : Division 5.2 - Organic peroxides, Handling Label - Keep Away  
From Heat  
Packing instruction (cargo aircraft) : 570  
Packing instruction (passenger aircraft) : 570

##### IMDG-Code

UN number : UN 3105  
Proper shipping name : ORGANIC PEROXIDE TYPE D, LIQUID  
(tert-BUTYL PEROXY-3,5,5-TRIMETHYLHEXANOATE)  
Class : 5.2  
Packing group : Not assigned by regulation  
Labels : 5.2  
EmS Code : F-J, S-R  
Marine pollutant : yes

#### Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

Hazchem Code : 2WE

#### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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### SECTION 15: Regulatory information

#### Safety, health, and environmental regulations specific for the hazardous chemical

Gefahrgruppe nach § 3 BGV B4: Ib (German regulatory requirements)

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Occupational Safety and Health (Classification, Labelling and Safety Data Sheet of Hazardous Chemicals) Regulations 2013.

Occupational Safety and Health (Use and Standards of Exposure of Chemicals Hazardous to Health) Regulations 2000.

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

TCSI (TW)	:	On the inventory, or in compliance with the inventory
TSCA (US)	:	All substances listed as active on the TSCA inventory
AICS (AU)	:	On the inventory, or in compliance with the inventory
DSL (CA)	:	All components of this product are on the Canadian DSL
ENCS (JP)	:	On the inventory, or in compliance with the inventory
ISHL (JP)	:	On the inventory, or in compliance with the inventory
KECI (KR)	:	On the inventory, or in compliance with the inventory
PICCS (PH)	:	On the inventory, or in compliance with the inventory
IECSC (CN)	:	On the inventory, or in compliance with the inventory
NZIoC (NZ)	:	On the inventory, or in compliance with the inventory

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## SECTION 16: Other information

### Further information

Other information	:	This safety datasheet only contains information relating to safety and does not replace any product information or product specification. These safety instructions also apply to empty packaging which may still contain product residues.
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Sources of key data used to compile the Safety Data Sheet	:	Internal technical data, data from raw material SDSs, OECD eChem Portal search results and European Chemicals Agency, <a href="http://echa.europa.eu/">http://echa.europa.eu/</a>
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Date format	:	dd.mm.yyyy
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### Full text of other abbreviations

AICS - Australian Inventory of Chemical Substances; ANTT - National Agency for Transport by Land of Brazil; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with

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x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECl - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; Nch - Chilean Norm; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NOM - Official Mexican Norm; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TDG - Transportation of Dangerous Goods; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative; WHMIS - Workplace Hazardous Materials Information System

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

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