

GPS Safety Summary

Substance Name:

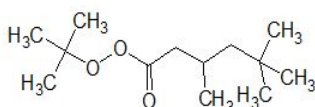
Tert-butyl 3,5,5-trimethylperoxyhexanoate

1. General Statement

Tert-Butyl 3,5,5-trimethylperoxyhexanoate is primarily used in the manufacture of polymers, as a polymerisation initiator.

2. Chemical Identity

Name:	Tert-butyl 3,5,5-trimethylperoxyhexanoate, tert-butyl peroxyisononanoate, TBPIN
Brand names:	Luperox® 270 grades, Link-Cup® TBPIN
Chemical name (IUPAC):	Tert-butyl 3,5,5-tris(methylperoxy)hexanoate
CAS number:	13122-18-4
EC number:	236-050-7
Molecular formula:	C ₁₃ H ₂₆ O ₃
Structure:	



3. Use and applications

Tert-Butyl peroxy-2-ethylhexanoate is primarily used as a radical initiator to induce polymerisation (free radical polymerisation process), for the manufacture of e.g. polyethylene, acrylic polymers, and as a curing agent for the production of unsaturated polyester resins.

4. Physical / Chemical properties

Property	Value
Physical state	Liquid at 20°C and 1013 hPa
Colour	colourless to slightly yellow
Odour	Slight, ester-like
Molecular weight	230.3 g/mol
Density	0.89 g/cm ³ at 20°C
Vapour pressure	0.03 hPa at 30°C
Melting point	- 69.15°C at 1013 hPa
Self-Accelerating Decomposition Temperature (SADT)	60°C

Oxidising properties	Not relevant, as the substance is an organic peroxide
Explosive properties	Non explosive
Water solubility	14.2 mg/L at 20°C
Octanol-water partition coefficient (Log K _{ow})	5.16 at 20°C

5. Health Effects

Effect Assessment	Result
Acute Toxicity Oral / inhalation / dermal	Based on the available data, no acute toxic effects
Irritation / corrosion Skin / eye/ respiratory tract	Slightly irritating for eye. Not irritating for skin
Sensitisation	Product may cause allergic skin reaction
Toxicity after repeated exposure Oral / inhalation / dermal	Based on the available test data, did not cause significant target organ toxicity after oral repeated exposure
Genotoxicity / Mutagenicity	Based on the available test data, it is not possible to conclude for gene mutation effects, since an <i>in vitro</i> test was positive.
Carcinogenicity	No data available
Reproductive / Developmental Toxicology	Based on the available test data, did not cause adverse effects on reproduction after oral exposure.

6. Environmental Effects

Effect Assessment	Result
Aquatic Toxicity	Very toxic to aquatic life

Fate and behaviour	Result
Biodegradation	Inherently biodegradable.
Bioaccumulation potential	Potentially bioaccumulative
PBT / vPvB conclusion	Not considered as PBT nor vPvB

7. Exposure

7.1 Human health

The manufacture of TBPIN is a closed process that occurs behind anti-deflagration walls, which minimizes worker exposure during the production process.

However, workers can be exposed during loading/unloading operations, mixing, sampling or maintenance operations.

The primary routes of industrial/professional exposure of TBPIN are skin contact and inhalation.

In addition, general population is not expected to be exposed to TBPIN by inhalation, dermal or oral exposure, the product does not remain in the plastic products.

Based on the risk assessment, risk is controlled when activities are carried out under conditions recommended in the extended safety data sheet (chapter 8 and exposure scenarios).

7.2 Environment

Releases of TBPIN into the environment are to be expected during production, processing (formulation) and industrial/professional uses mainly via wastewater and lesser amounts via emissions of vapour or powder (due to its physical state and its vapour pressure).

Potential release during production is treated by on-site and off-site risk management measures.

TBPIN is used for production of polymers and resins, which can be either dry or wet processes. In case of wet processes, releases to water have to be directed to a wastewater treatment plant.

The substance is used in low quantity in polymer/resin production, and is almost totally consumed during the process. Therefore the release to the environment is very low and, in spite of the environmental hazard profile of the substance, the use is considered as safe for the environment (which has been confirmed by a quantitative risk assessment performed in the framework of REACH regulation).

8. Risk Management recommendations

Human health measures	
Eye/Face protection	Safety glasses/goggles Half-mask during the discharge
Skin protection	Protective suit
Hand protection	Gloves: nitrile rubber, neoprene (suitable gloves tested to EN374)
Respiratory protection	Suitable respiratory equipment in case of insufficient ventilation, and for activities >1h
Organizational measures	Ensure workers are duly trained to minimize exposure
Engineering control	Provide sufficient air exchange and/or exhaust ventilation in work rooms
Environmental measures	
Can be discarded as waste water, when in compliance with local regulations. Do not spread sludge on natural soils. Eliminate the product by incineration after dilution in a suitable flammable solvent (in accordance with local and national regulations) – amount of active oxygen must be below 1%.	

9. Regulatory Information / Classification and Labelling

9.1 Regulatory Information

A dossier was generated by the Organic Peroxide Producers Association during the High Production Volume Program.




On top of that, the substance has been registered under EU Regulation EC 1907/2006 (REACH).

As organic peroxides are sensitive substances (as they are liable to exothermic decomposition), the transport of TBPEH is strongly regulated, under the rules and conditions of class 5.2 of UN Recommendations on the Transport of Dangerous Goods regulation.

%	Form	UN Number	Classification	OP Category
>32%-100%	liquid	UN 3105	OP Type D, Liquid, no temperature control	Type D: (i) detonates partially, does not deflagrate rapidly, no violent effects when heated under confinement; or (ii) does not detonate at all, deflagrates slowly, no violent effects when heated under confinement; or (iii) does not detonate or deflagrate, medium effect when heated under confinement
≤32%	liquid	UN 3109	OP Type F, Liquid, no temperature control	Type F: neither detonates in the cavitated state nor deflagrates at all and shows only a low or no effect when heated under confinement as well as low or no explosive power

9.2 Classification and labelling

Under GHS substances are classified according to their physical, health, and environmental hazards. The hazards are communicated via specific labels and the eSDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemicals in use. Substances registered for REACH are classified according CLP (EC) 1272/2008, implementation of the GHS in the European Union.

Classification	
According to REGULATION (EC) no 1272/2008:	
<ul style="list-style-type: none"> – Organic peroxide; type D; Heating may cause a fire. – Skin sensitization; Category 1B; May cause an allergic skin reaction. – Acute aquatic toxicity; Category 1; Very toxic to aquatic life. – Chronic aquatic toxicity; Category 1; Very toxic to aquatic life with long lasting effects. 	
Pictogram	
– GHS02: Flame	
– GHS07: Exclamation mark	
– GHS09: Environment	

Hazard statement
<ul style="list-style-type: none"> – H242: Heating may cause a fire. – H317: May cause an allergic skin reaction. – H410: Very toxic to aquatic life with long lasting effects.
Alternative classification according to Globally Harmonized System (GHS)
None.

10. Contact Information within Company

For further information on this substance or product safety summary in general, please contact:

- arkema.peroxides-reach-uses@arkema.com
- **ICCA portal where the GPS Safety Summary is posted:**
<http://www.icca-chem.org/en/Home/ICCA-initiatives/global-product-strategy/>

11. Date of Issues / Revision

- Date of issue: 2013/03/11
- Date of revision:

12. Disclaimer

The information contained in this paper is intended as advice only and whilst the information is provided in utmost good faith and has been based on the best information currently available, is to be relied upon at the user's own risk.

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