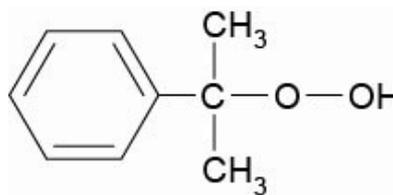


Trigonox K-90 PG

Cumyl hydroperoxide



Trigonox® K-90 PG is an organic peroxide (90% active ingredient in aromatic solvent mixture) for Asymmetric Oxidation and other pharmaceutical synthesis reactions.

CAS number
80-15-9

EINECS/ELINCS No.
201-254-7

TSCA status
listed on inventory

Molecular weight
152.2

Active oxygen content
peroxide
10.51%

Specifications

Acetophenone	≤ 2.0 %
Active oxygen	9.14-9.46 %
Appearance	Clear liquid
Assay	87.0-90.0 %
Color	≤ 200 Pt-Co
Cumene	≤ 8.0 %
Phenyl isopropanol	* ≤ 10.0 %
pH	4.0-7.0

Characteristics

Density, 20°C	1.06 g/cm ³
Viscosity, 20°C	10.4 mPa.s

Notes:

* Phenyl isopropanol = Cumyl alcohol

Applications

Trigonox® K-90 PG may be used in chemical synthesis of medicines and fine chemicals to make personal care and pharmaceutical products. The high purity and extensive compliance controls make it a low risk reagent or late stage intermediate. It can be used in emulsion, solution and bulk reactions and reactions are used in many blockbuster drugs.

Half-life data

The reactivity of an organic peroxide is usually given by its half-life ($t_{1/2}$) at various temperatures. The half-life of Trigonox® K-90 PG in chlorobenzene is:

0.1 hr	at 195°C
1 hr	at 166°C
10 hr	at 140°C
Formula 1	$k_d = A \cdot e^{-E_a/RT}$
Formula 2	$t_{1/2} = (\ln 2) / k_d$
Ea	132.56 kJ/mole
A	1.15E+12 s ⁻¹
R	8.3142 J/mole-K
T	(273.15+°C) K

Thermal stability

Organic peroxides are thermally unstable substances, which may undergo self-accelerating decomposition. The lowest temperature at which self-accelerating decomposition of a substance in the original packaging may occur is the Self-Accelerating Decomposition Temperature (SADT). The SADT is determined on the basis of the Heat Accumulation Storage Test.

SADT	75°C
Method	The Heat Accumulation Storage Test is a recognized test method for the determination of the SADT of organic peroxides (see Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria - United Nations, New York and Geneva).

Storage

Due to the relatively unstable nature of organic peroxides a loss of quality can be detected over a period of time. To minimize the loss of quality, Nouryon recommends a maximum storage temperature (T_s max.) for each organic peroxide product.

T_s max.	40°C
T_s min.	-30°C *
Note	* to prevent crystallization. When stored under these recommended storage conditions, Trigonox® K-90 PG will remain within the Nouryon specifications for a period of at least 3 months after delivery.

Packaging and transport

Trigonox® K-90 PG is packed in a 200 kg HDPE drums. Both packaging and transport meet the international regulations. For the availability of other packed quantities contact your Nouryon representative. Trigonox® K-90 PG is classified as Organic peroxide type F; liquid, Division 5.2; UN 3109.

Safety and handling

Keep containers tightly closed. Store and handle Trigonox® K-90 PG in a dry well-ventilated place away from sources of heat or ignition and direct sunlight. Never weigh out in the storage room. Avoid contact with reducing agents (e.g. amines), acids, alkalis and heavy metal compounds (e.g. accelerators, driers and metal soaps). Please refer to the Safety Data Sheet (SDS) for further information on the safe storage, use and handling of Trigonox® K-90 PG. This information should be thoroughly reviewed prior to acceptance of this product. The SDS is available at nouryon.com/sds-search

Major decomposition products

Acetophenone, 2-Phenylisopropanol, Methane

Additional information

This product is: allergen free, TSE/BSE compliant, has no elemental impurities, no genotoxic impurities, no genetic material impurities, melamine free, and contains no metallic catalyst residue.

All information concerning this product and/or suggestions for handling and use contained herein are offered in good faith and are believed to be reliable. Nouryon, however, makes no warranty as to accuracy and/or sufficiency of such information and/or suggestions, as to the product's merchantability or fitness for any particular purpose, or that any suggested use will not infringe any patent. Nouryon does not accept any liability whatsoever arising out of the use of or reliance on this information, or out of the use or the performance of the product. Nothing contained herein shall be construed as granting or extending any license under any patent. Customer must determine for himself, by preliminary tests or otherwise, the suitability of this product for his purposes. The information contained herein supersedes all previously issued information on the subject matter covered. The customer may forward, distribute, and/or photocopy this document only if unaltered and complete, including all of its headers and footers, and should refrain from any unauthorized use. Don't copy this document to a website.

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The logo for Nouryon, featuring a stylized blue 'N' followed by the word 'ouryon' in a blue sans-serif font.