Justification for the selection of a candidate CoRAP substance

Substance Name (Public Name):	2,5-di-tert-pentylhydroquinone
Chemical Group:	Organic
EC Number:	201-222-2
CAS Number:	79-74-3
Submitted by:	UK CA
Published:	20/03/2013

NOTE

This document has been prepared by the evaluating Member State given in the CoRAP update.

Contents

1 IDENTITY OF THE SUBSTANCE

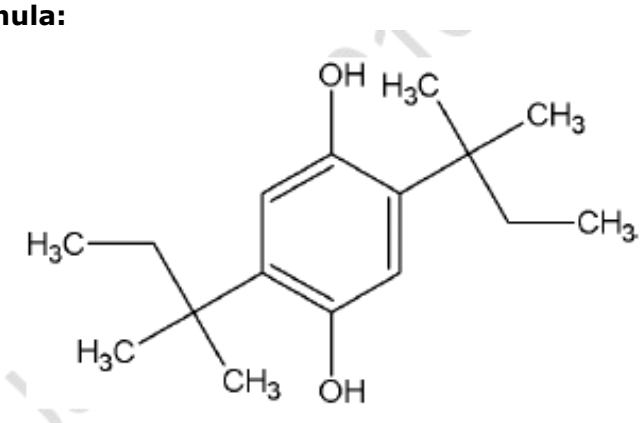
1.1 Name and other identifiers of the substance

Table 1: Substance identity

Public Name:	2,5-di-tert-pentylhydroquinone
EC number:	201-222-2
EC name:	2,5-di-tert-pentylhydroquinone
CAS number (in the EC inventory):	79-74-3
CAS number:	79-74-3
CAS name:	1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-
IUPAC name:	
Index number in Annex VI of the CLP Regulation	Not listed
Molecular formula:	$C_{16}H_{26}O_2$
Molecular weight or molecular weight range:	250.38 g/mol
Synonyms:	*Lowinox AH25; and* *Santovar A*

Type of substance ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

Structural formula:



2 CLASSIFICATION AND LABELLING

2.1 Harmonised Classification in Annex VI of the CLP

The substance is not listed

2.2 Proposal for Harmonised Classification in Annex VI of the CLP

No proposal has been submitted.

2.3 Self classification

The following self-classification by the registrants is published on the ECHA dissemination site.

CLP:

Acute Tox. 4 H302: Harmful if swallowed.

Aquatic Acute 1 H401: Toxic to aquatic life.

Aquatic Chronic 1 H410: Very toxic to aquatic life with long lasting effects.

DSD:

Xn; R22: Harmful if swallowed.

N; R50/53: Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Classification and labelling Inventory additionally includes the following classifications:

Aquatic Acute 1 H400 very toxic to aquatic life.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2 H319 Causes serious eye irritation.

Skin Sens. 1 H317 May cause an allergic skin reaction.

3 JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

3.1 Legal basis for the proposal

☒ Article 44(1) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

3.2 Grounds for concern

☐ (Suspected) CMR	☐ Wide dispersive use	☐ Cumulative exposure
☐ (Suspected) Sensitiser	☐ Consumer use	☒ High RCR
☒ (Suspected) PBT	☐ Exposure of sensitive populations	☐ Aggregated tonnage
☐ Suspected endocrine disruptor	☐ Other (provide further details below)	

PBT

The substance fulfils the P screening criterion: in the one available ready biodegradability test (OECD 301B, using a 10 day pre-adaptation period) 1% degradation after 28 d was observed. No information on any primary degradation is available.

No measure of bioaccumulation is available. There is some question over whether the B screening criteria are fulfilled. The registration data present a log Kow (OECD 117 HPLC method) of 3.3 (few details given). However, QSAR estimate of log Kow is much higher than this (KOWWIN v1.68 estimate = 5.83). The HPLC method may have been used as it appears that the water solubility was lower than the detection limit for the analytical method for the substance in water (< 0.08 mg/l) (note that the measured log Koc value was 3.68 (OECD 121)). No toxicokinetic investigations have been undertaken for human health.

The T screening criteria are fulfilled, and T itself is almost certainly fulfilled. Fish are the most sensitive species with a 96h LC_{50} of 0.013mg/l in bluegill (OECD 203, based on nominal concentrations). Four other acute studies are available in bluegill, fathead minnow and rainbow trout (2 studies): 96h LC_{50}s of 0.034, 0.04, 0.047 and 0.12 mg/l respectively, all based on nominal concentrations. No long term studies available.

High RCR

An exposure assessment and risk assessment for the environment has been carried out. Specific risk management measures (RMMs) taken from the CEFIC library are listed for some uses in the registration data. Nonetheless, RCRs for the environment for two uses are near parity for freshwater and sediment compartments (PNEC based on the acute fish result), and similar numbers are given for the marine environment.

3.3 Information on aggregated tonnage and uses

☐ 1 – 10 tpa	☒ 10 – 100 tpa	☐ 100 – 1000 tpa
☐ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ > 10,000,000 tpa	
☐ Confidential		

Tonnage banding given on the ECHA dissemination site.

☒ Industrial use	☒ Professional use	☐ Consumer use	☐ Closed System

Industrial use;

Manufacture of 2,5-bis(1,1-dimethylpropyl)benzene-1,4-diol,
Use as anti-oxidant in medium/high voltage cross-linked PE cables
Formulation of aqueous dispersions (polymer preparations)
Use as anti-oxidant in adhesives
Use as stabilizer in uncured rubber
Use as stabilizer in printing paper

Professional use;

Use as a laboratory reagent

Consumer use;

Use of adhesives

3.4 Other completed/ongoing regulatory processes that may affect suitability for substance evaluation

☐ Compliance check final decision	☐ Dangerous substances Directive 67/548/EEC
☒ Testing proposal	☐ Existing Substances Regulation 793/93/EEC
☐ Annex VI (CLP)	☐ Plant Protection Products Regulation 91/414/EEC
☐ Annex XV (SVHC)	☐ Biocidal Products Directive 98/8/EEC
☐ Annex XIV (Authorisation)	☐ Other (provide further details below)
☐ Annex XVII (Restriction)	

Following agreement of a testing proposal, a 90-day study in rats (oral administration) is being conducted.

3.5 Information to be requested to clarify the suspected risk

☐ Information on toxicological properties	☒ Information on physico-chemical properties
☒ Information on fate and behaviour	☒ Information on exposure
☒ Information on ecotoxicological properties	☐ Information on uses
☐ Other (provide further details below)	

PBT

Each of the three aspects could be investigated further: there are some indications that substances of this type (di-alkyl substituted phenols) may be subject to (primary) degradation in the environment; either the log Kow could be revisited and/or a BCF test conducted (assuming a suitable analytical technique can be derived); a long term toxicity study in fish with analytical confirmation of exposure concentrations could be conducted. The possibility of read across from other substances would be explored first before advocating vertebrate testing.

High RCR

In the first instance further information on actual releases from relevant uses would need to be sought, and possibly some kind of check made that identified RMMs were being put in place by downstream users, having been suitably identified in the eSDS. Should such information lead to a concern, further information might be necessary to refine the PNEC (and if so this would be considered in concert with the data needs for the PBT assessment).

3.6 Potential follow-up and link to risk management

☐ Restriction	☐ Harmonised C&L	☐ Authorisation	☐ Other (provide further details)

Given the complexity of the concerns identified for this substance, it is currently difficult to identify what, if any, follow-up will be necessary.