# Annex 15 Report
# Proposal for identification of a substance of very high concern (SVHC)

## Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP)

EC Number: -

CAS Number: -

**July 2026**

# Contents

# 1. Proposal

**Substance name**: Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP)

**EC number(s):** n/a (List number[1]**:** 700-960-7)

**CAS number(s):** n/a

OAPP is a UVCB (substance of Unknown or Variable composition, Complex reaction products and or Biological Materials). It contains a number of constituents, including a combination of mono-, di-, and tri-alkylated phenols and hydrocarbon resin from the oligomerisation of 2-phenylpropene. Oligomerisation results in isomeric constituents, including dimers and trimers, that can display either an inner or internal olefin moiety or intramolecular alkylation. The relative content of each constituent depends on the production method and desired commercial application (refer to Section 2 for full details).

OAPP has been identified as a substance of very high concern (SVHC) in accordance with the requirements set out in Annex 15 of EU REACH (ECHA, 2023a). This is based on the substance fulfilling the very persistent and very bioaccumulative (vPvB) criteria under Annex 13 of EU REACH.

This technical report provides an independent scientific assessment by the Agency[2] on whether OAPP should be identified as an SVHC under UK REACH. It considers only studies presented in the equivalent document produced by the European Chemicals Agency (ECHA), the EU Member State Committee (MSC) support document (ECHA, 2023b). Relevant observations on studies made in the support document have been summarised and Agency comments have been added where appropriate. Unpublished study reports were not available and have not been examined, unless stated otherwise. A literature search was not performed because the existing information is considered to be sufficient for decision making.

It is proposed to identify OAPP as vPvB according to Article 57(e) of UK REACH.

**Summary of how the substance meets the criteria set out in Article 57 of the REACH Regulation**

Based on the evidence presented in ECHA (2023b) a weight-of-evidence determination according to the provisions of Annex 13 of UK REACH has been used to identify OAPP as vPvB.

[1] A list number is an administrative identifier assigned by the European Chemicals Agency (ECHA) under REACH or CLP to substances that do not have official EC numbers.

[2]The Health and Safety Executive (HSE) acting in its capacity as the Agency for UK REACH, and with support from the Environment Agency in accordance with Article 2B of UK REACH.

*Persistence*

The evidence for persistence presented in this assessment is summarised as follows:

- Estimated biodegradation data from BIOWIN v4.10 indicate the dimer and trimer components of OAPP are potentially persistent (P) and very persistent (vP).
- Reliable studies demonstrate that both OAPP and the representative dimer 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (CAS no. 6362-80-7) do not fulfil the criteria to be considered readily biodegradable, with degradation values between 0% and 4% after 28 days and are therefore potentially P or vP.
- The degradation half-lives of the dimer 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8) from an OECD TG 309 aerobic mineralisation study are both considerably longer than the study length of 60 days, with one statistically reliable half-life of 205 days.

The Agency concludes that the dimer 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8) fulfils both the P and vP criteria of Annex 13 of UK REACH.

A read-across case is made that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) will experience similar or lower degradation compared to the dimer 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8). This is based on:

- Structural similarity between the trimer and the dimer, noting that the trimer includes an additional 2-phenylpropyl moiety at a site that is susceptible to degradation in the dimer, effectively eliminating this degradation site in the trimer.
- Similarity in estimated physicochemical properties such as water solubility and log $K_{OW}$ indicating both substances to be lipophilic.
- Evidence from estimated data that the susceptibility to biodegradation of the trimer is similar or lower than the dimer.
- Lower likelihood of degradation based on probable degradation pathways.

The Agency concludes, based on this read across, that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) fulfils the P and vP criteria of Annex 13 of UK REACH.

*Bioaccumulation*

The evidence for bioaccumulation for the dimers presented in this assessment is summarised as follows:

- The dimers screen as bioaccumulative (B) and very bioaccumulative (vB) based on log $K_{OW}$ values greater than 4.5 and predicted bioconcentration factor (BCF) values that were mostly above 2,000 L/kg.
- In an aqueous exposure OECD TG 305 using *Cyprinus carpio* (Common carp), BCF values for the dimer 1,1′-(1,1-dimethyl-3-methylene-1,3-propanediyl)-bisbenzene ranged from 368 to 5,208 L/kg.

- In a dietary OECD TG 305 study using *Pimephales promelas* (Fathead minnow), estimated BCF values for the dimers ranged from 499 to 4,608. For each dimer, 8 of the 13 estimation methods produced BCF values exceeding 2,000 L/kg.
- The growth-corrected depuration rate constant ($k_2$) from the dietary OECD TG 305 study (0.130 $day^{-1}$) meets the critical threshold of ≤ 0.178 $day^{-1}$ for a BCF ≥ 2,000 L/kg.

Therefore, the Agency concludes that the dimers fulfil the B criterion of Annex 13 of UK REACH.

The evidence for bioaccumulation for the trimers presented in this assessment is summarised as follows:

- The trimers screen as B/vB as log $K_{OW}$ values are greater than 4.5.
- Predicted laboratory BCF values were not considered relevant due to the hydrophobic nature of the trimers and that it is unlikely that they will be taken up directly from water.
- Predicted field bioaccumulation factor (BAF) values, which considered uptake from the diet as well as from water ranged from 15,810 to 177,800, indicating the likely relative importance of uptake via diet.
- A dietary bioaccumulation study conducted to OECD TG 305 with *P. promelas* (Fathead minnow) indicated that all of the trimers had calculated BCF values that exceeded the vB criterion (11 out of 13 estimation methods) by a considerable margin.
- The $k_2$ for the trimers (0.027 $d^{-1}$) from the dietary OECD TG 305 study meets the critical thresholds of ≤ 0.178 $day^{-1}$ for a BCF ≥ 2,000 L/kg and ≤ 0.085 $day^{-1}$ for a BCF ≥ 5,000 L/kg. This is consistent with other substances that have a high level of bioaccumulation.

The Agency concludes from the evidence available that the trimers fulfil the vB criterion of Annex 13 of UK REACH.

*Conclusion*

The Agency concludes, based on the evidence available, that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) fulfils the vPvB criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(e) of UK REACH.

If a constituent, impurity or additive of a substance fulfils the PBT/vPvB properties, a ≥ 0.1 % (w/w) threshold applies for concluding the substance as fulfilling the same criteria (ECHA, 2023c). Based on the information available, the Agency concludes that OAPP fulfils the vPvB criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(e) of UK REACH when containing the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane above or equal to 0.1% (w/w).

# 2. Justification

## 2.1 Identity of the substance and physical and chemical properties

### 2.1.1 Name and other identifiers of the substance

**Table 1: Substance identity**

| | |
|---|---|
| EC number: | Not applicable (List number[1]: 700-960-7) |
| List[1] name: | Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol |
| SMILES[a] | Not applicable (UVCB) |
| CAS no.: | Not applicable |
| IUPAC name: | Not applicable |
| Index number in GB Mandatory Classification and Labelling (MCL) List[c]: | No mandatory classification |
| Molecular formula: | Not applicable (UVCB) |
| Molecular weight range: | 212 to 449 g/mol |
| Synonyms: | Phenol, methylstyrenated<br>OAPP |
| Structural formula: | Not applicable (UVCB) |

[a] SMILES: Simplified Molecular Input Line Entry System
[b] IUPAC: International Union of Pure and Applied Chemistry
[c] GB MCL list in accordance with the retained Regulation (EC) No 1272/2008 as amended for Great Britain

The substance has previously been identified with the name phenol, methylstyrenated with EC number 270-966-8 and CAS number 68512-30-1.

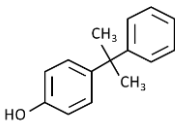
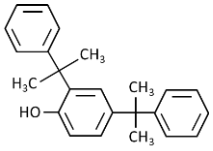
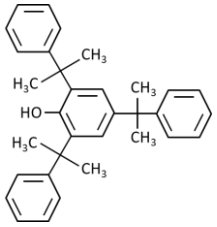
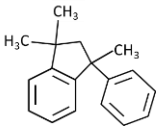
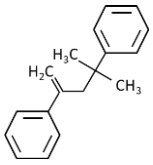
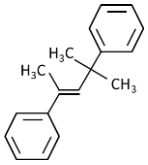
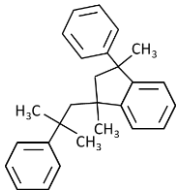
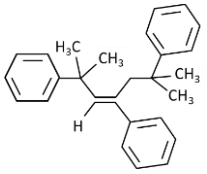
### 2.1.2 Composition of the substance

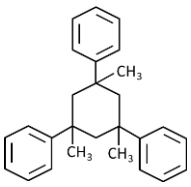
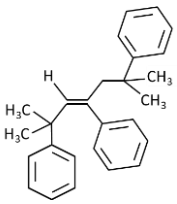
**Substance type:** UVCB

OAPP consists of a combination of mono-, di-, and tri-alkylated phenols and hydrocarbon resin from the oligomerisation of 2-phenylpropene. Oligomerisation results in isomeric constituents, including dimers and trimers, that can display either an inner or internal olefin moiety or intramolecular alkylation. The relative content of each constituent depends on the production method and desired commercial application. The EU REACH registration

dossiers contain information on the concentration ranges of the constituents; however, this is considered confidential information and as such was not provided in ECHA (2023b). No information on composition is available for any products on the UK market. Table 1 presents the general substance information for OAPP reproduced from ECHA (2023b). Table 2 presents constituents other than impurities/additives presented in ECHA (2023b).

**Table 2: Constituents other than impurities/additives presented in ECHA (2023b)**

| Substance | Identifiers | Type | Structural formula |
|---|---|---|---|
| 4-(α,α-dimethylbenzyl)phenol | EC no. 209-968-0<br>CAS no. 599-64-4 | Monoalkylated phenol |  |
| 2,4-bis(1-methyl-1-phenylethyl)phenol | EC no. 220-466-0<br>CAS no. 2772-45-4 | Dialkylated phenol |  |
| 2,4,6-tris(1-methyl-1-phenylethyl)phenol | EC no. 250-325-9<br>CAS no. 30748-85-7 | Trialkylated phenol |  |
| 1,1,3-trimethyl-3-phenylindane | EC no. 223-467-4<br>CAS no. 3910-35-8 | Dimer |  |
| 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene | EC no. 228-846-8<br>CAS no. 6362-80-7 | Dimer |  |
| 1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene | EC no. 228-396-2<br>CAS no. 6258-73-7 | Dimer |  |
| 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindane | EC no. 255-584-1<br>CAS no. 41906-71-2 | Trimer |  |
| 1,1',1"-[(3E)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene | EC no. not available<br>CAS no. not available | Trimer |  |

| Substance | Identifiers | Type | Structural formula |
|---|---|---|---|
| 1,3,5-triphenyl-1,3,5-trimethylcyclohexane | EC no. not available<br>CAS no. not available | Trimer |  |
| 1,1',1"-[(3Z)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene | EC no. not available<br>CAS no. 957070-06-3 | Trimer |  |

### 2.1.3 Identity and composition of transformation products relevant for the SVHC assessment

No transformation products were considered in ECHA (2023b). The Agency has not considered any transformation products as part of this assessment.

### 2.1.4 Identity and composition of structurally related substances (used in grouping or read-across approach)

The assessment presented in ECHA (2023b) includes relevant data for the dimers and trimers. No consideration was given to the alkylated phenols as they were not considered relevant to SVHC identification.

The Agency has only considered the dimers and trimers and not the alkylated phenols nor any additional structurally related substances.

### 2.1.5 Physicochemical properties

OAPP is made up of a number of constituents with a range of physicochemical properties. Table 3 details properties for OAPP reported in the EU registration dossier (ECHA, 2010) and reproduced in ECHA (2023b).

ECHA (2023b) also reported predicted values for log $K_{OW}$ (KOWWIN v1.68), water solubility (WATERNT v1.01), and vapour pressure (MPBPWIN v1.43), using the models available in EPISuite™™ (US EPA, 2023) for the dimer and trimers (Table 4). It notes that the dimers and trimers were within the molecular weight range of the training dataset for KOWWIN and WATERNT but that the complete training set for MPBPWIN was not available.

**Table 3: Overview of physicochemical properties of OAPP presented in ECHA (2023b)**

| Property | Value |
|---|---|
| Physical state at 20°C and 101.3 kPa | Colourless liquid, viscous with slight phenolic odour. |
| Melting/freezing point (°C) at 101.2 kPa | -14<br>No decomposition or sublimation was noted. |
| Boiling point (°C) at 101.2 kPa | > 300<br>No decomposition was noted. |
| Vapour pressure (Pa) | 20°C: 0.03 to 0.06<br>100°C: 22<br>200°C: 3,030 |
| Water solubility (mg/L) | 0.5 to 7 mg total organic carbon (C)/L at 20 to 25°C<br>Solubility is loading dependant.<br>At loadings of 100 mg/L, the water-accommodated fractions amounted to 1.5 to 4 mg C/L |
| n-Octanol–water partition coefficient (log $K_{OW}$) (25°C) | 3.6 to > 6.3 |
| Dissociation constant ($pK_a$, 20°C) | Not applicable |
| Viscosity (25°C) | 100 mPa s to 1,200 mPa s depending on composition |

**Table 4: Overview of physicochemical properties for the dimer and trimers as presented in ECHA (2023b); estimated values from EPISuite™™ v4.11 unless stated**

| Substance | CAS number | Molecular weight (g/mol) | Water solubility (mg/L) | Vapour pressure (Pa at 25°C) | Log $K_{OW}$ |
|---|---|---|---|---|---|
| Dimers | | | | | |
| 1,1,3-trimethyl-3-phenylindane[a] | 3910-35-8 | 236 | 0.0339 | 0.0924 | 5.91 |
| 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene[b] | 6362-80-7 | 236 | 0.0384 | 0.0303 | 6.51<br>6.2 (measured) |
| 1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene[c] | 6258-73-7 | 236 | 0.0820 | 0.0233 | 6.43 |
| Trimers | | | | | |
| 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindane[d] | 41906-71-2 | 355 | $1.248 \times 10^{-4}$ | $5.58 \times 10^{-6}$ | 8.98 |
| 1,1',1"-[(3E)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene[e] | - | 355 | $4.45 \times 10^{-5}$ | $6.47 \times 10^{-6}$ | 9.5 |
| 1,3,5-triphenyl-1,3,5-trimethylcyclohexane[f] | - | 355 | $5.05 \times 10^{-5}$ | $3.99 \times 10^{-6}$ | 9.44 |
| 1,1',1"-[(3Z)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene[g] | 957070-06-3 | 355 | $4.45 \times 10^{-5}$ | $6.47 \times 10^{-6}$ | 9.5 |

SMILES codes sourced by the Agency from PubChem – [a] CC1(CC(C2=CC=CC=C21)(C)C3=CC=CC=C3)C; [b] CC(C)(CC(=C)C1=CC=CC=C1)C2=CC=CC=C2; [c] C/C(=C/C(C)(C)C1=CC=CC=C1)/C2=CC=CC=C2; [d] CC1(CC(C2=CC=CC=C21)(C)C3=CC=CC=C3)CC(C)(C)C4=CC=CC=C4; [e] (Z)-2,6-Dimethyl-2,4,6-triphenylhept-3-ene - (C(C)(C/C(=C/C(C)(C)C1=CC=CC=C1)/C2=CC=CC=C2)C3=CC=CC=C3; [f] CC1(CC(CC(C1)(C)C2=CC=CC=C2)(C)C3=CC=CC=C3)C4=CC=CC=C4; [g] (Z)-2,6-Dimethyl-2,4,6-triphenylhept-3-ene - CC(C)(C/C(=C/C(C)(C)C1=CC=CC=C1)/C2=CC=CC=C2)C3=CC=CC=C3.

The Agency notes that using data from more than one QSAR or estimation method would be preferable because each approach is developed from different training sets, chemical domains, and underlying assumptions, all of which influence prediction outcomes. In addition, the algorithms themselves can work very differently, for example, fragment-based methods estimate properties by summing the contributions of molecular substructures, whereas free energy or regression based relationships rely on thermodynamic principles and global molecular descriptors. No single method can capture all aspects of chemical behaviour, so comparing multiple QSARs helps balance method-specific biases. Agreement between methods increases confidence in the results, while divergence highlights uncertainty, leading to more robust and scientifically defensible conclusions.

## 2.2 Mandatory classification and labelling

OAPP is not listed on the GB mandatory classification and labelling (MCL) list nor on Annex 6 of Regulation (EC) No 1272/2008.

## 2.3 Environmental fate properties

### 2.3.1 Degradation

#### 2.3.1.1 Abiotic degradation

The information on abiotic degradation presented in ECHA (2023b) is summarised in Table 5. It concludes that primary photodegradation in air is likely to be rapid but that the trimers may be sorbed to airborne particles to a larger extent than the dimers and therefore could be more resistant to photodegradation. Also, the support document states that distribution to air is predicted to be very low and therefore this degradation pathway is likely to be of minor importance.

**Table 5: Summary of abiotic degradation data presented in ECHA (2023b)**

| Abiotic degradation process | Information available | Results |
|---|---|---|
| Hydrolysis | No experimental data | OAPP is composed of constituents that do not contain functional groups susceptible to hydrolysis under environmental conditions |
| Oxidation | No information available for OAPP | - |
| Phototransformation in air | Predicted using AOPWIN v1.92 (US EPA, 2023). | Dimers:<br>• Half-life for reaction with hydroxyl radicals (at 25°C) = 0.11 to 0.99 days (12-hour day; 1.5 × $10^6$ OH/$cm^3$)<br>• Half-life for reaction with ozone (at 25°C) = 0.08 days (at 7 × $10^{11}$ mol/$cm^3$)[a].<br>• Fraction sorbed to airborne particulates: 0.00054 to 0.002<br>Trimers:<br>• Half-life for reaction with hydroxyl radicals (at 25°C) = 0.11 to 0.61 days (12-hour day; 1.5 × $10^6$ OH/$cm^3$)<br>• Half-life for reaction with ozone (at 25°C) = 0.08 days (at 7 × $10^{11}$ mol/cm3)[b].<br>• Fraction sorbed to airborne particulates: 0.77 to 0.89. |

[a] No ozone reaction estimation available for 1,1,3-trimethyl-3-phenylindane.
[b] No ozone reaction estimation available for 1,3-dimethyl-1-(2 methyl-2-phenylpropyl)3-phenylindane or 1,3,5-triphenyl-1,3,5 trimethylcyclohexane.

### 2.3.1.2 Biodegradation

#### *2.3.1.2.1 Biodegradation in aqueous media*

##### *2.3.1.2.1.1 Estimated data*

Estimated biodegradation data from BIOWIN v.4.10 reported in ECHA (2023b), are summarised in Table 6. On applicability domain, the support document states that the molecular weights of the dimers and trimers fall within the training set range of the models.

**Table 6: BIOWIN v4.10 predicted results for BIOWIN models 2, 3, and 6; from ECHA (2023b)**

| Group | Substance | BIOWIN (v.4.10)[a] | | |
|---|---|---|---|---|
| | | BIOWIN 2 | BIOWIN 3 | BIOWIN 6 |
| Dimers | 1,1,3-trimethyl-3-phenylindane | 0.12 | 2.28 | 0.11 |
| | 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene | 0.82 | 2.51 | 0.10 |
| | 1,1'-(1,3,3-trimethylprop-1 ene-1,3-diyl)dibenzene | 0.82 | 2.51 | 0.07 |
| Trimers | 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindane | 0.03 | 1.82 | 0.001 |
| | 1,1',1"-[(3E)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | 0.48 | 2.06 | 0.003 |
| | 1,3,5-triphenyl-1,3,5-trimethylcyclohexane | 0.14 | 1.85 | 0.001 |
| | 1,1',1"-[(3Z)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | 0.48 | 2.06 | 0.003 |

[a] A substance screens as potentially P or vP if the values generated for BIOWIN 2 or BIOWIN 6 are < 0.5 and values generated for BIOWIN 3 are < 2.25 (between 2.25 and 2.75 more information is required to draw a conclusion) (ECHA, 2023c).

##### *2.3.1.2.1.2 Screening tests*

Four ready biodegradability studies are reported in ECHA (2023b). One study assessed 4-(α,α-dimethylbenzyl)phenol (EC no. 209-968-0, CAS no. 599-64-4). However, as this substance is an alkylated phenol and therefore falls outside the scope of the current assessment, it was not considered further by the Agency. The other three studies are summarised in Table 7.

ECHA (2023b) assigns the study conducted according to OECD Test Guideline (TG) 310 as reliable without restrictions, because the validity criteria of the guideline were met. The study conducted according to OECD TG 301C was considered reliable with restrictions, as although the validity criteria of the test were fulfilled, specifically, oxygen uptake in the inoculum blank was below 60 mg $O_2$/L after 28 days, and aniline degradation reached 53% after 7 days and 66% after 14 days, limitations were identified, notably that the test

substance remained undissolved. In contrast, the study conducted according to OECD TG 302B was not assigned a reliability score, as information on toxicity, lag phase, and pre-adaptation was not provided, and the result of the aniline reference test was not reported. In addition, the exposure concentration exceeded the water solubility.

**Table 7: Screening test results for OAPP (EC no. 700-960-7) and the dimer 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC no. 228-846-8; CAS no. 6362-80-7) presented in ECHA (2023b)**

| Reference | Study details | Results |
|---|---|---|
| Unpublished (2010) | Equivalent to OECD TG 310<br>Activated sludge (domestic).<br>OAPP at 23.7 mg/L<br>28 days<br>Reliable without restrictions | OAPP: 4% degradation after 28 days (by $CO_2$ evolution) |
| Unpublished (2002) | 28-day OECD TG 301C<br>Non-adapted activated sludge.<br>Dimer (CAS no. 6362-80-7) at 100 mg/L<br>Reliable with restrictions | 0% degradation after 28 days (by oxygen consumption)<br>3% primary degradation (by HPLC analysis) |
| Unpublished (2013) | 28-day OECD TG 302C.<br>Mixed population of active sludge micro-organisms from 10 sites in the UK.<br>Dimer (CAS no. 6362-80-7) at 30 mg/L)<br>Reliability not assignable | By oxygen consumption:<br>18% degradation after 14 days<br>64% degradation after 28 days<br>Primary degradation:<br>82% after 28 days |

The Agency concludes that there was no evidence from these studies to demonstrate that OAPP or the dimer (1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)-bisbenzene; CAS no. 6362-80-7) are readily biodegradable. Data for the dimer in an OECD 302C (inherently biodegradable test) showed considerable degradation but the threshold of ≥70% mineralisation (oxygen uptake) was not met. The Agency considers that this result should be treated with caution as the reliability of study is uncertain.

*2.3.1.2.1.3 Biodegradation (aqueous simulation tests)*

ECHA (2023b) provides information for one aerobic mineralisation simulation study conducted to OECD TG 309, for the dimer 1,1,3-trimethyl-3-phenylindane as test substance (summarised in Table 8).

**Table 8: Summary of biodegradation data for the dimer 1,1,3-trimethyl-3-phenylindane (EC no. 223-467-4, CAS no. 3910-35-8) presented in ECHA (2023b)**

| Reference | Study details | Results |
|---|---|---|
| Unpublished (2022) | 60-day OECD TG 309 at 12°C. River water (Devon, UK). $^{14}$C-radiolabelled dimer, 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8) at 1 and 10 µg/L<br><br>Reliable without restrictions | Mineralisation of up to 11.2% (peak at day 28) and 10.6% (peak at day 14) for 1 and 10 µg/L, respectively.<br><br>$DT_{50}$ values: 542 and 205 days at 1 and 10 µg/L, respectively.<br><br>One main metabolite identified as 1,3-dimethyl-3-phenyl-2,3 dihydro-1H-indene-1-carboxylic acid. |

- Unpublished (2022)

The validity criteria of the study were fulfilled as the reference substance (benzoic acid) reached 77% degradation after 14 days and the total recovery of applied radioactivity (AR) was generally between 90 and 110%. ECHA (2023b) noted that the test substance was present at greater than 90% and 75% AR after 60 days, at the 1 and 10 µg/L exposure concentrations, respectively. Kinetic assessments of the degradation data were conducted using CAKE v3.4. Fittings using single first order kinetics resulted in $DT_{50}$ values of 542 and 205 days for the test concentrations of 1 and 10 µg/L, respectively. However, the degradation rate (k) value for 1 µg/L was not significantly different from zero. The statistically unacceptable fitting for 1 µg/L is likely because of insufficient data to adequately model very limited degradation. This outcome may be explained through additional scrutiny of mass balance data, taking into consideration the high log $K_{OW}$ of the test substance in aqueous only media. Ultimately, the Agency concludes that the half-life at this concentration is considerably longer than 60 days but that a specific value cannot be assigned.

#### 2.3.1.3 Persistence read across from dimers to trimers

ECHA (2023b) presents a case for read across of the conclusion for persistence from the dimer, 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8), to the trimer, 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2). Several strands of evidence are presented:

- Similarity in physicochemical properties: Although there are no measured values, predicted water solubility was low and predicted log $K_{OW}$ values relatively high, indicating both substances are expected to be lipophilic. This is supported by the predicted water solubility of the dimer being greater than that of the trimer and predicted log $K_{OW}$ being lower for the dimer compared to the trimer (see

- Table 4).
- Structural similarity: the trimer includes an additional 2-phenylpropyl moiety at a site that is susceptible to degradation in the dimer, effectively eliminating this degradation site in the trimer. The trimer is therefore likely to be at least as persistent as the dimer.
- Computational evidence: BIOWIN v4.10 model data (see Table 6) indicates a susceptibility to biodegradation for the trimer similar to or potentially lower than for the dimer. ECHA (2023b) also presents computational analysis using the CATALOGIC 301C model (OASIS LMC, 2022) that predicts primary and ultimate half-lives concluding that the dimer and trimer are potentially P or vP . The Agency confirmed the EPISuite™ numeric values presented but cannot verify those from the CATALOGIC model.
- Probable degradation pathways: The CATALOGIC model predicted a lower probability of methyl group hydroxylation for the trimer compared to the dimer (the probable observed degradation pathway observed in the OECD TG 309 study for the dimer).

ECHA (2023b) concludes that the evidence discussed above is acceptable to support the read-across hypothesis that the trimer 1,3-dimethyl-1-(2-methyl-2- phenyl)propyl-3-phenylindane is at least as persistent as the dimer 1,1,3-trimethyl-3-phenylindane. The Agency agrees with this conclusion because the dimers and trimers are structurally similar with the same functional groups present and that the weight of evidence presented indicates that the trimer is likely to be more persistent than the dimer.

#### 2.3.1.4 Summary and discussion of degradation

The degradation of dimers and trimers present in OAPP is predicted to be slow.

Reliable studies demonstrated that both OAPP and the representative dimer 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (CAS no. 6362-80-7) did not meet the threshold to be considered readily biodegradable, with degradation values between 0% and 4% after 28 days. Considerable mineralisation (68%) was observed for the dimer in the inherently biodegradable study, although this did not meet the 70% threshold; interpretation of these data should be treated with caution due to the study being unassignable for reliability.

A single simulation study conducted in accordance with OECD TG 309 (reliable without restrictions) provided direct evidence of degradation behaviour for the dimer 1,1,3-trimethyl -3-phenylindane. The study demonstrated slow degradation with half-lives considerably longer than the study length of 60 days at both test concentrations, including a statistically reliable half-life of 205 days at 10 µg/L.

Using a read-across argument, the structurally similar trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane is expected to have a lower rate of biodegradation than the dimer.

## 2.3.2 Bioaccumulation

### 2.3.2.1 Bioaccumulation in aquatic organisms

#### *2.3.2.1.1 Screening data*

All dimers and trimers have estimated log $K_{OW}$ values exceeding 4.5 (Table 4).

ECHA (2023b) reports data from the BCFBAF and Arnot-Gobas models in EPISuite™ (Table 9) noting that the dimers and trimers are within the applicability domain of the models. The predicted laboratory fish BCFs are mostly in the range 2,200 to 9,200 for the dimers (one model predicts a BCF of 1,700 for one of the dimers), with higher values predicted by the BCFBAF model.

The BAFBCF model is based on the relationship between log $K_{OW}$ and experimental BCF values from aqueous uptake studies; experimental BCF values peak in relation to a substance log $K_{OW}$ of 7 and then decrease. Consequently, the high estimated log $K_{OW}$ values of the trimers (8.98 to 9.5) lead to expected lower predicted BCFs than for the dimers, with values in the range 750 to 1,420. The Arnot-Gobas BCF mechanistic model considers uptake from the water at the gill surface and produced even lower predicted BCF values for the trimers, suggesting that aqueous uptake via the gills may be a less important route for the trimers than for the dimers.

By contrast, the Arnot-Gobas mechanistic model for bioaccumulation factor (BAF) calculation includes both uptake at the gills and from the diet. Predicted BAFs are higher than BCFs for both the dimers and the trimers, and exceed 10,000 for all but one substance, indicating the likely relative importance of uptake via the diet.

**Table 9: Predicted BCF and BAF values for the dimers and trimers presented in ECHA (2023b)**

| Group | Substance | Predicted BCF and BAF values |
|---|---|---|
| Dimers | 1,1,3-trimethyl-3-phenylindane | BCFBAF (BCF): 3,681<br>Arnot-Gobas (BCF): 2,482<br>Arnot-Gobas (BAF): 7,388 |
| | 1,1'-(1,1-dimethyl-3-methylene-1,3- propanediyl)bisbenzene | BCFBAF (BCF): 9,201<br>Arnot-Gobas (BCF): 1,711<br>Arnot-Gobas (BAF): 13,730 |
| | 1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene | BCFBAF (BCF): 8,165<br>Arnot-Gobas (BCF): 2,241<br>Arnot-Gobas (BAF): 21,760 |
| Trimers | 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindane | BCFBAF, BCF: 1,426<br>Arnot-Gobas (BCF): 113<br>Arnot-Gobas (BAF): 177,800 |
| | 1,3,5-triphenyl-1,3,5-trimethylcyclohexane | BCFBAF (BCF): 849<br>Arnot-Gobas (BCF): 21 |

| Group | Substance | Predicted BCF and BAF values |
|---|---|---|
| | | Arnot-Gobas (BAF): 15,810 |
| | 1,1',1"-[(3E)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | BCFBAF, BCF: 789<br>Arnot-Gobas (BCF): 41<br>Arnot-Gobas (BAF): 76,540 |
| | 1,1',1"-[(3Z)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | BCFBAF, BCF: 789<br>Arnot-Gobas (BCF): 41<br>Arnot-Gobas (BAF): 76,540 |

#### *2.3.2.1.2 Laboratory studies*

ECHA (2023b) reports two bioaccumulation studies which are briefly summarised in Table 10.

**Table 10: Summary of aquatic bioaccumulation data from ECHA (2023b)**

| Reference | Study detail | Results |
|---|---|---|
| Unpublished (2002) | Flow-through aqueous exposure OECD TG 305 using *Cyprinus carpio* (Common carp) using 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (CAS no. 6362-80-7) at 1 and 10 µg/L.<br>Uptake phase: 60 days<br>Depuration phase: 16 days<br>BCF values as a ratio of concentration in fish and water<br>Reliable with restrictions | BCF (1 µg/L): 404 to 4,691 L/kg<br>BCF (10 µg/L): 368 to 5,208 L/kg<br>All values after lipid normalisation. No growth correction was applied |
| Unpublished (2017) | Flow-through dietary exposure OECD TG 305. *Pimephales promelas* (Fathead minnow).<br>OAPP (concentration in the food): 0.39 mg/g for dimers, 0.23 mg/g for trimers.<br>Uptake phase: 14 days<br>Depuration phase: 28 days<br>BCF ranges from OECD BCF estimation tool<br>Reliable without restrictions | Growth-corrected depuration rate constant ($k_{2g}$):<br>Dimers: 0.130 $d^{-1}$<br>Trimers: 0.027 $d^{-1}$ |

- Unpublished (2002)

ECHA (2023b) reports an aqueous bioaccumulation study conducted in accordance with a protocol equivalent to OECD Test Guideline (TG) 305:

- The study was performed within the framework of the Japanese Existing Chemicals Survey by the National Institute of Technology and Evaluation (NITE, 2002b). In this study, *Cyprinus carpio* (Common carp) with a mean body length of 8 ± 4 cm were exposed to 1,1′-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC No. 228-846-8; CAS No. 6362-80-7).
- Fish were exposed under flow-through conditions for 60 days at nominal concentrations of 1 µg/L and 10 µg/L, followed by a depuration phase of 16 days. The exposure was conducted at 24 ± 2°C, with dissolved oxygen concentrations maintained at ≥ 60 % air saturation. Prior to the test, fish were acclimated for at least two weeks, during which mortality did not exceed 5 % over a 7 day period. Measured concentrations of the test substance in the exposure water were maintained within ± 20 % of the mean measured values throughout the uptake phase.
- No mortality or treatment-related abnormalities were observed during either the uptake or depuration phases. The lipid content of the fish was determined at the start of exposure, and at the end of the uptake and depuration phases. Concentrations of the test substance in both fish tissue and test media were analytically determined on a weekly basis using gas chromatography–mass spectrometry (GC/MS). Method recoveries ranged from 95.8 % to 108.3 %, and the limit of detection was 0.05 µg/L. It is noted that the sampling intervals have not been presented in ECHA (2023b)
- The study was assessed as reliable with restrictions. This was because steady state was not achieved, as the average BCF values varied by more than 20 % across three consecutive sampling points; therefore, a steady state BCF ($BCF_{SS}$) could not be derived. No data relating to the mass or growth of the fish, husbandry, or total organic carbon concentrations have been presented.
- BCF values were calculated as the ratio of the measured concentration in fish to that in water during the uptake phase. These yielded BCF values ranging from 427 to 3,330 for the high exposure group (10 µg/L) and from 423 to 4,410 for the low exposure group (1 µg/L).
- BCF values normalised to a lipid content of 4 % were also reported in the study. When recalculated to a standard lipid content of 5 %, these lipid normalised BCFs ($BCF_L$) ranged from 368 to 5,208 for the 10 µg/L group and from 404 to 4,691 for the 1 µg/L group. No correction for growth dilution was applied, as there is no reliable method for such correction, in line with OECD TG 305 and Brooke and Crookes (2012).

- Unpublished (2017)

ECHA (2023b) reports a dietary bioaccumulation study with OAPP in *Pimephales promelas* (Fathead minnow) in accordance with OECD Test Guideline (TG) 305 (Bioaccumulation in Fish: Aqueous and Dietary Exposure), combined with elements of OECD TG 229 (Fish Short-Term Reproduction Assay) for the measurement of vitellogenin:

- The study was performed under flow-through conditions and consisted of a 14-day uptake phase followed by a 28-day depuration phase. During the uptake phase, five fish were sampled on days 0, 7 and 14. During the depuration phase, five fish were sampled on days 1, 2, 5, 8, 15, 21 and 28. Additionally, three samples of the feed were collected and analysed on days 1, 7 and 14 of the uptake phase (spiked food) and on day 4 of the depuration phase (un-spiked food). No information was reported regarding the homogeneity of the test substance in the spiked food. There was no verification of non-contamination with OAPP in the un-spiked food.
- Growth rates of 0.0073 $day^{-1}$ and 0.0045 $day^{-1}$ were reported for the control and test group, respectively. No lipid data are presented in ECHA (2023b), although confirmation of lipid correction for the values is provided.
- The nominal concentration in the food was 250 µg/g for the reference substance hexachlorobenzene (HCB), with analytical recoveries of 81–108%; 100 µg/g for 17β-estradiol, with recoveries of 99–105%; 0.39 mg/g for the dimers, with recoveries of 81–83%; and 0.23 mg/g for the trimers, with recoveries of 90–107%.
- Water temperature was monitored continuously, and at three time points during the study hourly measurements indicated temperatures below the target range of 21 ± 2 °C. These deviations were considered minor and not to have adversely affected the integrity of the study. Dissolved oxygen concentrations remained stable throughout the test and ranged between 80 % and 100 % air saturation.
- In both the test and control groups, no significant mortality or non-lethal adverse effects were observed, with a cumulative mortality of 0.6 % after 42 days. In contrast, the reference test(s) conducted with HCB, and 17β-estradiol resulted in elevated mortality, with cumulative mortality reaching 18.2 % between days 10 and 42. In addition, internal bleeding was observed in some fish during the uptake phase of the reference test.
- As the inclusion of a reference test is not a requirement of OECD TG 305, and the main dietary bioaccumulation study fulfilled all validity criteria specified in the guideline, the study was considered valid. Overall, the study was assessed as reliable without restriction.

Although the study analytically quantified three individual dimer constituents and seven individual trimer constituents, ECHA (2023b) presents the results as aggregated concentrations, expressed as total dimers and total trimers. Substance-specific bioaccumulation metrics were therefore not directly derived for the individual components.

Briefly, ECHA (2023b) reports for the dimers and trimers:

- growth corrected BMF values ($BMF_{kg}$) values of 0.042 and 0.078, respectively.
- growth and lipid corrected BMF values ($BMF_{kgL}$) of 0.074 and 0.137, respectively.
- growth-corrected depuration rate constants ($k_2$) of 0.130 $d^{-1}$ and 0.027 $d^{-1}$, respectively. These values were independently verified by the Agency.

ECHA (2023b) notes that the $k_2$ values were used as input parameters to the OECD BCF estimation tool to derive bioconcentration factor (BCF) estimates. On this basis, a range of BCF values was calculated for three dimer constituents and four trimer constituents present in OAPP, extrapolating from the experimentally derived depuration behaviour of the aggregated dimer and trimer fractions. The use of aggregated dimer and trimer data introduces uncertainty into the component-specific BCF estimates, as potential differences in uptake and depuration kinetics between individual constituents cannot be resolved.

The estimated BCF values were also checked by the Agency, and a summary of the results is presented in Table 11.

**Table 11: BCF values from the OECD BCF estimation tool (total number of BCF values = 14), summarised from ECHA (2023b)**

| Group | Substance | BCF estimations | | |
|---|---|---|---|---|
| | | BCF Range | Estimated BCFs above 2,000 | Estimated BCFs above 5,000 |
| Dimers | 1,1,3-trimethyl-3-phenylindane | 499 to 3,982 | 8 | 0 |
| | 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene | 502 to 4,330 | 8 | 0 |
| | 1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene | 471 to 4,608 | 8 | 0 |
| Trimers | 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindane | 121 to 46,952 | 2 | 11 |
| | 1,1',1"-[(3E)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | 67 to 55,987 | 2 | 11 |
| | 1,3,5-triphenyl-1,3,5-trimethylcyclohexane | 71 to 54,862 | 2 | 11 |
| | 1,1',1"-[(3Z)-2,6-dimethylhept-3-ene-2,4,6- triyl]tribenzene | 67 to 55,987 | 2 | 11 |

With respect to the numerical BCF estimates, the predicted BCF values for the dimers exceeded 2,000 in 8 out of 13 estimation methods, although none exceeded 5,000. For the trimers, predicted BCF values exceeded 2,000 in 2 methods and exceeded 5,000 in 11 out of 13 methods; notably, all but one of the values above 5,000 were also above 10,000.

ECHA (2023b) notes that, for the trimers, the predicted log $K_{OW}$ values slightly exceeded the upper applicability domain of two of the OECD BCF estimation methods; and that one estimation method developed specifically for carp was identified as not applicable to the dietary study data. Despite these methodological limitations, the support document emphasises that the majority of estimated BCF values for the trimers were substantially above the regulatory criteria value of 5,000, indicating very high bioaccumulation potential irrespective of model domain constraints.

The Agency notes that excluding the estimated laboratory BCF values on the basis of model applicability domain considerations would disproportionately affect the highest predictions for the trimers and would therefore underestimate their bioaccumulation potential.

ECHA (2023b) provides a comparison of the growth corrected depuration rate constant for the trimers (0.027day$^{-1}$) with that of HCB (0.06 day$^{-1}$), a well-characterised persistent organic pollutant (POP), and concludes that depuration of the trimers is slower than that of HCB, implying a higher tendency for retention in fish tissue. This observation is consistent with the Agency's evaluation of the experimentally derived $k_2$ which were 0.130 day$^{-1}$ for the dimer fraction and 0.027 d$^{-1}$ for the trimer fraction. Both values are below the critical $k_2$ thresholds presented in Brooke and Crookes (2012) as indicators of bioaccumulation potential e.g. BCF ≥ 2,000; $k_2$ ≤ 0.178 day$^{-1}$. The growth-corrected $k_2$ value for the trimers (0.027 d$^{-1}$) is also below the critical value proposed for very bioaccumulative (vB) substances ($k_2$ ≤ 0.085 day$^{-1}$; BCF ≥ 5,000), providing independent kinetic support for a vB conclusion.

#### 2.3.2.2 Summary and discussion of bioaccumulation

The dimers of OAPP are potentially bioaccumulative based on estimated log $K_{OW}$ values that are all greater than 4.5. Predicted laboratory BCF values using the BCFBAF and Arnot-Gobas models ranged from 1,711 to 9,201 with five of the six values above 2,000. The range of BCF values for the dimer 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene was 368 to 5,208 L/kg in a laboratory study equivalent to OECD TG 305 (reliable with restrictions). The BCF values for the dimers from a dietary OECD TG 305 study which tested the whole OAPP substance (rated reliable without restrictions) calculated with the OECD BCF estimation tool ranged from 499 to 4,608 L/kg, with values above 2,000 in 8 of the 13 methods for each dimer.

The trimers of OAPP also have estimated log $K_{OW}$ values above 4.5, but these are close to or above 9. Predicted BCFs consequently range from 21 to 1,426, which are generally much lower than for the dimers. This is because the BCFBAF model predicts a drop off in BCF values for substances with very high log $K_{OW}$ values and because the Arnot-Gobas BCF model only considers uptake from the water at the gill surface. The Arnot-Gobas BAF model considers uptake from gills and diet and predicted high BAF values for both dimers and trimers indicate the potential importance of dietary exposure.

The BCF values for the trimers from the dietary OECD TG 305 study (rated reliable without restrictions) calculated with the OECD BCF estimation tool were above 5,000 in 11 of the 13 methods (and above 2,000 in 2 more).

Importantly, even when accounting for applicability domain limitations, the convergence of evidence from (i) the remaining high BCF estimates, (ii) the consistently low empirical depuration rate constants, and (iii) the comparison with a benchmark POP such as HCB indicates that the overall conclusion of high to very high bioaccumulation potential for the trimers is robust. Omission of those values would not change the interpretation but would increase uncertainty by narrowing the quantitative basis of the assessment. Overall, there is evidence that significant bioaccumulation occurs for both the dimers and the trimers. The trimers are likely to be more bioaccumulative than the dimers with uptake of trimers primarily from food and not from water.

## 2.4 Conclusions on the SVHC properties

### 2.4.1 PBT and vPvB assessment

#### 2.4.1.1 Persistence

The evidence for persistence presented in Section 2.0 of this assessment is summarised as follows:

- The values presented from BIOWIN v4.10 indicate that the selected dimer and trimer components of OAPP are potentially P or vP. All components screen as potentially P or vP with the values for BIOWIN 2 or BIOWIN 6 < 0.5 and values generated for BIOWIN 3 are < 2.25.
- OAPP and the representative dimer 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (CAS no. 6362-80-7) did not meet the threshold to be considered readily biodegradable, with degradation values between 0% and 4% after 28 days in reliable studies. The dimer achieved a high degree of mineralisation in an inherent degradability study of unknown reliability but did not exceed the > 70% threshold. They therefore screen as potentially P or vP.
- The surface water degradation half-lives of the dimer at 1 and 10 µg/L 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8) from an OECD TG 309 aerobic mineralisation study are both considerably longer than the study length of 60 days with one statistically reliable half-life of 205 days (10 µg/L).

The Agency concludes that the dimer 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8) fulfils both the P and vP criteria under UK REACH Annex 13 (i.e. the degradation half-life in fresh water is higher than 40 days (P) and 60 days (vP)).

A read-across case is made that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) will experience similar or lower degradation compared to the dimer 1,1,3-trimethyl-3-phenylindane (CAS no. 3910-35-8). This is based on:

- Similarity in estimated physicochemical properties such as water solubility and log $K_{OW}$ indicating both substances to be lipophilic.
- Structural similarity of the trimer to the dimer as the trimer has an addition of a 2-phenylpropyl moiety at a susceptible point for chemical reaction (removing this potential site of degradation in the trimer)
- Evidence from estimated data that the susceptibility to biodegradation of the trimer is similar to or lower than the dimer
- Lower likelihood of degradation based on probable degradation pathways

The Agency concludes, based on this read across, that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) fulfils the P and vP criteria of Annex 13 of UK REACH.

#### 2.4.1.2 Bioaccumulation

The evidence for bioaccumulation for the dimers presented in this assessment is summarised as follows:

- The dimers screen as potentially B/vB based on log $K_{OW}$ values greater than 4.5.
- Predicted BCF values were mostly above 2,000 L/kg.
- The range of BCF values for the dimer 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene was 368 to 5,208 L/kg in an aqueous exposure bioaccumulation study equivalent to OECD TG 305, using *Cyprinus carpio* (Common carp) as the test species. Steady state was not achieved in the study.
- The range of BCF values for the dimers from a fully reliable dietary OECD TG 305 study with *P. promelas* was 499 to 4,608 L/kg, with values above 2,000 L/kg in 8 of the 13 estimation methods for each dimer.
- The growth-corrected depuration rate constant ($k_2$) from the dietary OECD TG 305 study (0.130 $day^{-1}$) meets the critical threshold of ≤ 0.178 $day^{-1}$ for a BCF ≥ 2,000 L/kg.
- The majority of BCF values for the dimers estimated from the laboratory studies are greater than 2,000 L/kg, and this is supported by the predicted BCF values.

The Agency concludes that the dimers fulfil the B criterion of Annex 13 of UK REACH (BCF above 2,000 L/kg).

The evidence for bioaccumulation for the trimers presented in this assessment is summarised as follows:

- The trimers screen as potentially B/vB as log $K_{OW}$ values are all greater than 4.5.
- Predicted laboratory BCF values were not considered relevant due to the hydrophobic nature of the trimers and that it is unlikely that they will be taken up directly from water.

- Predicted field bioaccumulation factor (BAF) values, which considered uptake from the diet as well as from water ranged from 15,810 to 177,800, indicating the likely relative importance of uptake via diet
- The dietary bioaccumulation study conducted to OECD TG 305 with *P. promelas* (Fathead minnow) indicated that all of the trimers had BCF values that exceeded 5,000 L/kg (11 out of 13 estimation methods), typically by a considerable margin. The $k_2$ for the trimers (0.027 $d^{-1}$) from the dietary OECD TG 305 study meets the critical thresholds of ≤ 0.178 $day^{-1}$ for a BCF ≥ 2,000 L/kg and ≤ 0.085 $day^{-1}$ for a BCF ≥ 5,000 L/kg. This is consistent with other substances that have a high level of bioaccumulation.

The Agency concludes from the evidence available that the trimers fulfils the vB criterion of Annex 13 of UK REACH (BCF above 5,000 L/kg).

#### 2.4.1.3 Overall conclusions on the PBT and vPvB properties

The Agency concludes, based on the evidence available, that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane (CAS no. 41906-71-2) fulfils the vPvB criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(e) of UK REACH.

If a constituent, impurity or additive of a substance fulfils the PBT/vPvB properties a ≥ 0.1% (w/w) threshold applies for concluding the substance as fulfilling the same criteria (ECHA, 2023).

Based on the information available, the Agency concludes that OAPP fulfils the vPvB criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(e) of UK REACH when containing the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane above or equal to 0.1% (w/w).

# 3. Information on use, exposure and alternatives

## 3.1 UK and EU REACH registration status and tonnage

The substance is not registered under UK REACH. However, a total of 82 Downstream User Import Notifications (DUINs[3]) have been submitted. This includes 15 DUINs for the group using the ECHA List no. 700-960-7 and 67 for phenol methylstyrenated, an historical name for OAAP (EC no. 270-966-8; CAS no. 68512-30-1).

Under EU REACH, OAPP (List no. 700-960-7) is registered with an aggregated tonnage of 1000 – 10,000 tpa (3 active EU registrants). There are no registrations under EU REACH for phenol methylstyrenated (EC no. 270-966-8; CAS no. 68512-30-1).

## 3.2 General description of uses and exposure

OAPP is an additive used in the manufacture and formulation of rubber, polymers, coatings, adhesives, sealants and inks (ECHA, 2023a). It functions primarily as a stabiliser or performance additive, improving durability and resistance of materials to degradation. Products containing OAPP have a wide range of industrial, professional and consumer applications e.g., in machinery, vehicles, wood and wood products, pulp, paper and paper products, electrical and optical equipment, furniture and rubber products (ECHA, 2023a).

There is potential for OAPP to be released to the environment during manufacture and formulation of products containing the substance and from their subsequent use, including outdoor use of long life articles by consumers.

## 3.3 Alternatives

No information available.

[3] GB-based companies who imported substances from EU-based suppliers before UK REACH became law on 1 January 2021 had no EU REACH registration obligations as they were classed as Downstream Users (DUs). As they are now importers from outside of GB, they may have registration obligations under UK REACH. However, a transitional measure allows former DUs to suspend the registration until one of three deadlines (depending on tonnage and hazard). Where the identity of these imported substances was known, they could be included in a Downstream User Import Notification (DUIN) submitted to the Agency.

# References

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# Glossary

| | |
|---|---|
| **Agency, the** | HSE |
| **B** | Bioaccumulative |
| **BAF** | Bioaccumulation factor |
| **BCF** | Bioconcentration factor |
| **CAKE** | Computer Assisted Kinetic Evaluation |
| **CAS** | Chemical Abstracts Service |
| **$DT_{50}$** | Time taken for 50% decline in mass or concentration. If the decline is described by first order kinetics, then this is also called the half-life |
| **DU** | Downstream User |
| **DUIN** | Downstream User Import Notification |
| **ECHA** | European Chemicals Agency |
| **EC** | European Community |
| **EU** | European Union |
| **HCB** | Hexachlorobenene |
| **IUPAC** | International Union of Pure and Applied Chemistry |
| **$K_{ow}$** | n-Octanol–water partition coefficient |
| **MCL** | Mandatory classification and labelling |
| **MSC** | Member State Committee |
| **OECD** | Organisation for Economic Cooperation and Development |
| **P** | Persistent |
| **$pK_a$** | Acid dissociation constant (logarithmic form) |
| **POP** | Persistent organic pollutant |
| **REACH** | Registration, evaluation, authorisation and restriction of chemicals |
| **SFO** | Single first order |
| **SMILES** | Simplified Molecular Input Line Entry System |
| **SVHC** | Substance of very high concern |
| **TG** | Test guideline |
| **UK** | United Kingdom |

| | |
|---|---|
| **UVCB** | Unknown or Variable composition, Complex reaction product or Biological material |
| **vB** | Very bioaccumulative |
| **vP** | Very persistent |
| **vPvB** | Very persistent and very bioaccumulative |

## Further information

This publication is available on the HSE website here.



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