Substance Name: Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol

List Number: 700-960-7[1]

CAS Number: -

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF

OLIGOMERISATION AND ALKYLATION REACTION PRODUCTS OF 2-PHENYLPROPENE AND PHENOL

AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS VPVB (ARTICLE 57E) PROPERTIES

Adopted on 29 November 2023

[1] Explanation on the role of LIST numbers is provided in the ECHA website at: https://echa.europa.eu/information-on-chemicals/registered-substances/information

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ABBREVIATIONS

ACF: atom centred fragments
BAF: bioaccumulation factor
BCF: bioconcentration factor
CLP: classification, labelling and packaging
DegT50: degradation half-life
HCB: Hexachlorobenzene
HPLC: high-performance liquid chromatography
Kd: distribution coefficient
Koc: organic carbon-water partition co-efficient
Kow: n-Octanol/Water Partition coefficient
kM: metabolic rate
OECD: Organisation for Economic Cooperation and Development
POP: Persistent organic pollutant
UVCB: substance of unknown or variable composition, complex reaction products or biological materials
vPvB: very persistent and very bioaccumulative
SFO: single first-order
SVHC: substance of very high concern
TG: test guideline
QPRF: (Q)SAR Prediction Reporting Format
(Q)SAR: (quantitative) structure activity relationships

IDENTIFICATION OF A SUBSTANCE OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57

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

List number: 700-960-7

CAS number: -

- The substance is identified as very persistent and very bioaccumulative (vPvB) according to Article 57 (e) of Regulation (EC) No 1907/2006 (REACH).

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

A weight-of-evidence determination according to the provisions of Annex XIII of REACH has been used to identify the substance as vPvB. All available relevant information, such as the results of standard tests, monitoring and modelling, information from the application of the analogue approach (read-across) and (Q)SAR results, was considered together in a weight-of-evidence approach.

Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP) is a UVCB (substance of Unknown or Variable composition, Complex reaction products and or Biological Materials) consisting of a number of constituents. Some of these constituents are the result of the alkylation of phenols. Others are the result of the oligomerisation of 2-phenylpropene and display relatively similar structures. Within the oligomeric constituents, one of these constituent groups refers to the dimers of 2-phenylpropene, another, to the trimers of 2-phenylpropene.

Persistence

Very limited biodegradation (4% after 28 days) was observed in an OECD TG 310 ready biodegradation study (reliable without restriction) with the whole substance OAPP. Ready biodegradation tests are not capable of discriminating between the relative degradation of each of the constituents and it is hypothesised that strong sorption of some of the extremely lipophilic constituents may reduce the bioavailability to degrading microorganisms. A ready biodegradability test equivalent to OECD TG 301 C (reliable with restrictions) carried out with the dimer of 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7) indicates that the constituent screens as potentially P or vP (0-3% biodegradation after 28 days).

Reliable QSAR predictions for biodegradation (Biowin 2, Biowin 3 and Biowin 6) indicate that all dimers screen as potentially P or vP but more degradation relevant information is generally warranted. As regards the trimers, reliable QSAR predictions for biodegradation using Biowin 2, Biowin 3 and Biowin 6 indicate that all the trimer constituents screen as potentially P or vP.

A reliable without restriction OECD TG 309 test (Aerobic Mineralisation in Surface Water – Simulation Biodegradation Test) was performed on the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4; CAS 3910-35-8) which was chosen as a potential worst-case representative for the dimer fraction. [^{14}C] radiolabelled test material was used and the study conducted over 60 days at two concentrations, 1 and 10 µg/L, at 12 °C. After 60 days, 11.2% and 10.6% mineralisation was reached for the 1 and 10 µg/L concentrations, respectively. One main metabolite was identified in both experiments, 1,3-dimethyl-3-

phenyl-2,3-dihydro-1H-indene-1-carboxylic acid. The study indicates that the dimer 1,1,3-trimethyl-3-phenylindan fulfils the P/vP criteria with a half-life in freshwater ≥205 days.

No experimental data is available for the trimers, therefore a read-across approach was used based on the structural similarity between the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) supported with (Q)SAR results in a weight-of-evidence approach. Based on a read-across approach with the dimer, it can be reasonably assumed that the trimer is at least as persistent as the dimer and thus the degradation half-life in water of the trimer exceeds 60 days. As a consequence, it is concluded that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) is very persistent in water (degradation half-life >60 days) in accordance with REACH Annex XIII.

Since OAPP contains the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2) with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets both the 'persistence' (P) (degradation half-life in water > 40 days) and 'very persistent' (vP) (degradation half-life in water > 60 days) criteria in accordance with Annex XIII, points 1.1.1 (b) and 1.2.1 (a), of the REACH Regulation.

Bioaccumulation

The dimers and trimers both screen as potentially B and vB with log kow values > 4.5 based on QSAR estimates.

The dimers have shown a potential to reach high levels in fish, both in carp (aqueous OECD TG 305 study performed on CAS 6362-80-7; reliable with restrictions) and in the fathead minnow (dietary OECD TG 305 study performed on the whole substance; reliable without restrictions) where the BCF values ranged from 499—4608 depending on the estimation method (most above 2000). This accumulation is furthermore supported by (Q)SAR predictions.

As regards the trimers, the dietary OECD TG 305 (Bioaccumulation in Fish: Aqueous and Dietary Exposure) performed on the whole substance indicates BCF values above 10000 (values in the range of 66.5-55 987 depending on the estimation method). Due to the high hydrophobicity of the trimers, the (Q)SAR predictions support high accumulation in fish through uptake via food compared to uptake over the gills.

The trimers are within the applicability domain of the Arnot-Gobas QSAR model and the reliable prediction for the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is a BAF of 177 800, the highest of the trimers. Since 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is predicted to be the most bioaccumulative of the trimers and the OECD TG 305 dietary study indicates BCF values mostly above 10000, 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is considered to fulfil the vB criteria of REACH Annex XIII (BCF > 5000).

Since OAPP contains trimer constituents with B/vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

Conclusion

In conclusion, OAPP is identified as a vPvB substance according to Art. 57(e) of REACH by comparing all relevant and available information listed in Annex XIII of REACH with the criteria set out in the same Annex, in a weight-of-evidence determination. As documented in this report, the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2) present in this UVCB, fulfils the vP criteria as well as the vB criteria.

Registration dossiers submitted for the substance: Yes

Justification

1. Identity of the substance and physical and chemical properties

1.1 Name and other identifiers of the substance

Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP) is a UVCB (substance of Unknown or Variable composition, Complex reaction products or of Biological Materials) and can therefore not be described by unique structures and molecular formulas. It consists of a number of constituents. Some of these constituents are the result of the alkylation of phenols where the phenol can be monoalkylated, dialkylated and trialkylated. Others are the result of the oligomerisation of 2-phenylpropene and include dimers and trimers of relatively similar structures.

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

The alkylated phenols in OAPP are not considered relevant for this SVHC identification under Article 57 (e) of the REACH Regulation, and the focus in this dossier is accordingly on the dimers and trimers.

Table 1: Substance identity

List number:	700-960-7
List name:	Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol
CAS number:	-
Index number in Annex VI of the CLP Regulation	No harmonised classification
Molecular formula:	Not applicable (UVCB)
Molecular weight range:	212-449 g/mol
Synonyms:	*OAPP; phenol, methylstyrenated;*

Structural formula: UVCB (see Table 2)

1.2 Composition of the substance

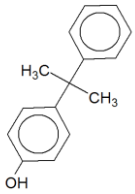
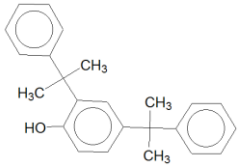
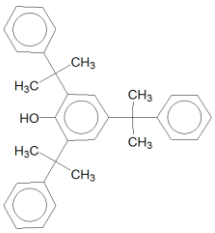
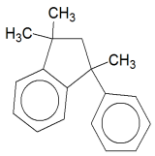
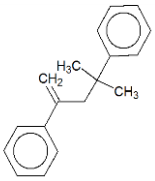
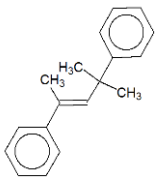
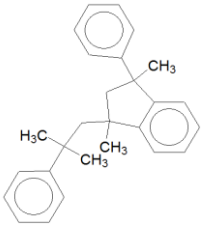
Name: Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP)

Description:

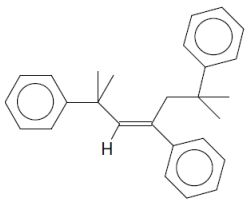
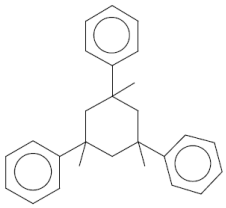
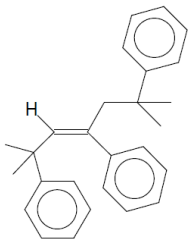
A combination of alkylated phenols and hydrocarbon resin from the oligomerisation of 2-phenylpropene. Based on the compositional information reported by the registrants of OAPP, the oligomerisation reaction results in constituents, including dimers and trimers, that can be available in different isomeric forms. They can display an inner or internal olefin moiety or they can have undergone an intramolecular alkylation. Table 2 provides information on the chemical nature of these constituents.

Substance type: UVCB[2]

Table 2: Constituents other than additives

Constituents	Structure	Concentration range
4-(*a,a*-dimethylbenzyl)phenol EC no.: 209-968-0 CAS no.: 599-64-4 Type: monoalkylated phenol		Confidential information
2,4-bis(1-methyl-1-phenylethyl)phenol EC no.: 220-466-0 CAS no.: 2772-45-4 Type: dialkylated phenol		Confidential information
2,4,6-tris(1-methyl-1-phenylethyl)phenol EC no. : 250-325-9 CAS no.: 30748-85-7 Type: trialkylated phenol		Confidential information
1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8 Type: dimer		Confidential information
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7 Type: dimer		Confidential information
1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7 Type: dimer		Confidential information
1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2 Type: trimer		Confidential information.

[2] Substances of Unknown or Variable composition, Complex reaction products or Biological materials

Constituents	Structure	Concentration range
1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene Type: trimer		Confidential information
1,3,5-triphenyl-1,3,5-trimethylcyclohexane Type: trimer		Confidential information
1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3 Type: trimer		Confidential information

Differences in production methods can lead to differences in composition with regard to the relative content of the different constituents that can be present in the composition of the substance, which again can be used to achieve different properties in the commercial products. The REACH registration dossiers contain information on concentration ranges of the constituents. However, this is considered as confidential business information by the registrants.

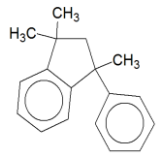
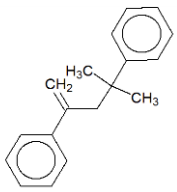
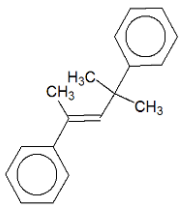
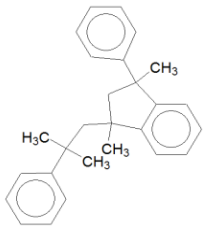
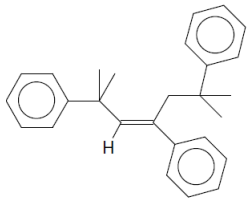
1.3 Physicochemical properties

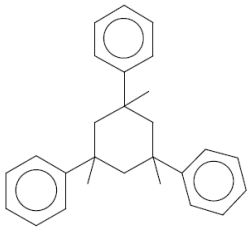
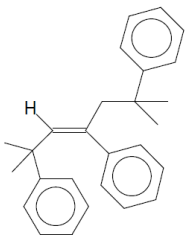
OAPP is a colourless viscous liquid at standard temperature and pressure. As a UVCB, the substance is composed of constituents with a range of physicochemical properties. The values reported in the registration dossiers are included in Table 3. In addition, predicted values for log Kow (KOWWIN v1.68), water solubility (WATERNT v1.01) and vapour pressure (MPBPVP v1.43), available in EPIsuite (US EPA, 2023), for the trimer and dimers are included in Table 4. For these models there are no universally accepted definition of model domain. The dimers and trimer are within molecular weight range of the training set for KOWWIN and WATERNT. The complete training sets for MPBPWIN's estimation methodology are not available.

Table 3: Overview of physicochemical properties

Property	Value	Remarks
Physical state at 20 °C and 101.3 kPa	At 20 °C and 1013 hPa the substance is a colourless viscous liquid with a slightly phenolic odour.	
Vapour pressure	At 20 °C the vapour pressure was between 0.03 and 0.06 Pa and between 0.06 at 25 °C. Vapour pressure at 100 °C was 22 Pa and at 200 °C 3030 Pa.	Multiple studies similar to OECD TG 104 have been performed with reliability ranging from reliability with restriction to not assignable (for the high temperature studies). Predicted values for the single constituents are provided in Table 4.
Water solubility	Due to the nature of the product there is a range of water solubilities. The range begins at 0.5 mg TOC/L and extends to 7 mg TOC/L between 20 and 25 °C, depending on the loading used. At loadings of 100 mg/L, the water-accommodated fractions amounted to 1.5 to 4 mg C/L, i.e. 1.5 to 4 %.	A number of OECD TG 105 studies (reliability with restriction) were conducted using the registered substance. Predicted values for the single constituents are provided in Table 4.
Partition coefficient n-octanol/water (Log Kow)	Due to the nature of the product there is a range of log Kow values. The range begins at 3.6 and extends to beyond 6.3 at 25 °C.	OECD TG 117 (reliable with restriction) and OECD TG 107 (reliable with restriction). Predicted values for the single constituents are provided in Table 4.
Stability in organic solvents and identity of relevant degradation products	Not applicable	The resin types of the substance are organic liquids miscible with other organic solvents without loss of stability.
Dissociation constant	Not applicable	The resin types of the substance contain only phenolic structures that are known to be very weak acids with typical pKa values in the range of 9.9 to 10.9
Viscosity	Due to the nature of the product there is a range of viscosities. The range begins at 100 mPa s and extends to 1200 mPa s at 25 °C.	National German test guideline DIN 53019 (rotational viscosimeter method) (reliable with restriction)
Melting/freezing point	Freezing point = -14 °C. No decomposition or sublimation was noted.	ISO 3016 test (reliable with restriction)
Boiling point	The start of the boiling point range is greater than 300 °C. No decomposition was noted.	DIN 51751 (reliable with restriction)

Table 4: Overview of physicochemical properties for the dimer and trimers

Constituent	Structure	Molecular weight	(Q)SAR (EPIsuite v4.11; US EPA, 2023)
1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8 Type: dimer		236	**Water solubility** 0.0339 mg/L **Vapour pressure** 0.0924 Pa (25 °C) **Log Kow** 5.91
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7 Type: dimer		236	**Water solubility** 0.0384 mg/L Measured 0.23 mg/L (20 °C) **Vapour pressure** 0.0303 Pa (25 °C) Measured 0.06 Pa (25 °C) **Log Kow** 6.51 Measured 6.2
1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7 Type: dimer		236	**Water solubility** 0.0820 mg/L **Vapour pressure** 0.0233 Pa (25 °C) **Log Kow** 6.43
1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2 Type: trimer		355	**Water solubility** 124.8 ng/L **Vapour pressure** 5.58*10^{-6} Pa (25 °C) **Log Kow** 8.98
1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene Type: trimer		355	**Water solubility** 44.5 ng/L **Vapour pressure** 6.47*10^{-6} Pa (25 °C) **Log Kow** 9.5

Constituent	Structure	Molecular weight	(Q)SAR (EPIsuite v4.11; US EPA, 2023)
1,3,5-triphenyl-1,3,5-trimethylcyclohexane Type: trimer		355	**Water solubility** 50.5 ng/L **Vapour pressure** 3.99*10^{-6} Pa (25 °C) **Log Kow** 9.44
1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3 Type: trimer		355	**Water solubility** 44.5 ng/L **Vapour pressure** 6.47*10^{-6} Pa (25 °C) **Log Kow** 9.5

2. Harmonised classification and labelling

OAPP is not listed in annex VI to the CLP Regulation. Neither are any of the constituents.

3. Environmental fate properties

3.1 Degradation

3.1.1 Abiotic degradation

3.1.1.1 Hydrolysis

OAPP is composed of constituents that do not contain functional groups susceptible to hydrolysis under environmental conditions. Hence, the substance is considered hydrolytically stable.

3.1.1.2 Oxidation

No information on oxidation is available for OAPP. In a hydrolysis-oxidation test (OECD TG 111) with the analogue UVCB phenol, styrenated only very limited degradation was observed and half-lives of 95 days (pH 7 buffer saturated with nitrogen) and 315 days (pH 7 buffer saturation with oxygen) were estimated (Brooke et al., 2009). Based on the composition of OAPP and the data on the analogue, oxidation of the dimers and trimers is unlikely.

3.1.1.3 Phototransformation/photolysis

3.1.1.3.1 Phototransformation in air

No information on photo transformation in air is available.

AOPWIN v1.92 (US EPA, 2023) estimations for the dimers and trimers are included in Table 5. Based on these estimates the constituents are considered to undergo primary degradation in the atmosphere via reaction with hydroxyl radicals. However, the trimers are predicted to be sorbed to airborne particulates to a high degree (77-89%). According to AOPWIN 'the sorbed fraction may be resistant to atmospheric oxidation'. Thus, the predicted half-lives are likely largely underestimating the half-life of the trimers in the atmosphere. Currently there is no universally accepted definition of model domain for AOPWIN and the complete training sets for AOPWIN's estimation methodology are not available.

Table 5: Predicted photo transformation in air

Group	Substance	Predicted photo transformation in air (AOPWIN v1.92)
Dimers	1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.99 days** (11.8 hours) (at 12-hour day; 1.5 x 10^6OH/cm^3) No ozone reaction estimation available Fraction sorbed to airborne particulates (koa): 0.00054
	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.18 days** (2.2 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). Half-life for reaction with ozone (at 25 °C) = **0.08 days** (at 7 x 10^{11} mol/cm^3). Fraction sorbed to airborne particulates (koa): 0.002
	1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.11 days** (1.4 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). Half-life for reaction with ozone (at 25 °C) = **0.08 days** (at 7 x 10^{11} mol/cm^3). Fraction sorbed to airborne particulates (koa): 0.00134
Trimers	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.64 days** (7.7 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). No ozone reaction estimation available Fraction sorbed to airborne particulates (koa): 0.77
	1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.11 days** (1.3 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). Half-life for reaction with ozone (at 25 °C) = **0.08 days** (at 7 x 10^{11} mol/cm^3). Fraction sorbed to airborne particulates (koa): 0.89
	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.61 days** (7.3 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). No ozone reaction estimation available Fraction sorbed to airborne particulates (koa): 0.89
	1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	Half-life for reaction with hydroxyl radicals (at 25 °C) = **0.11 days** (1.3 hours) (at 12-hour day; 1.5 x 10^6 OH/cm^3). Half-life for reaction with ozone (at 25 °C) = **0.08 days** (at 7 x 10^{11} mol/cm^3). Fraction sorbed to airborne particulates (koa): 0.89

3.1.1.3.2 Phototransformation in water

No information on phototransformation in water is available for OAPP and no information were identified for the individual constituents in a literature search.

3.1.1.3.3 Phototransformation in soil

No information on phototransformation in soil is available for OAPP and no information were identified for the individual constituents in a literature search.

3.1.1.4 Summary on abiotic degradation

The dimers are expected to undergo relatively rapid primary photodegradation in air based on their structure. The trimers are more resistant to photodegradation and may to a large extent not be photodegraded due to mainly being sorbed to airborne particulates.

The distribution to air of the dimers and trimers is predicted to be very low. Hence, unless release of the substance is directly to air, this degradation pathway appears to be of minor importance.

3.1.2 Biodegradation

3.1.2.1 Biodegradation in aqueous media or aqueous environment

3.1.2.1.1 Estimated data

Table 6: Predicted half-life in days in four different environmental compartments with PBT profiler (US EPA, 2002) and Biowin 2, 3 and 6 estimates (US EPA, 2023). Values exceeding screening criteria for "P" and thus potentially P or vP according to ECHA, 2017a are in bold.

Group	Substance	Predicted half-life (days) in different media (PBT profiler)		BIOWIN (v.4.10)		BIOWIN conclusion (ECHA R.11)
Dimers	1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	Water: Soil: Sediment: Air:	38 75 **340** 1.5	Biowin 2 Biowin 3 Biowin 6	**0.12** **2.28** **0.11**	Potentially P or vP*
	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	Water: Soil: Sediment: Air:	38 75 **340** 0.06	Biowin 2 Biowin 3 Biowin 6	0.82 **2.51** **0.10**	Potentially P or vP*
	1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	Water: Soil: Sediment: Air:	38 75 **340** 0.06	Biowin 2 Biowin 3 Biowin 6	0.82 **2.51** **0.07**	Potentially P or vP*
Trimers	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	Water: Soil: Sediment: Air:	**60** 120 **540** 0.96	Biowin 2 Biowin 3 Biowin 6	**0.03** **1.82** **0.001**	Potentially P or vP
	1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	PBT profiler not available		Biowin 2 Biowin 3 Biowin 6	**0.48** **2.06** **0.003**	Potentially P or vP

Group	Substance	Predicted half-life (days) in different media (PBT profiler)	BIOWIN (v.4.10)		BIOWIN conclusion (ECHA R.11)
	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	PBT profiler not available	Biowin 2 Biowin 3 Biowin 6	**0.14** **1.85** **0.001**	Potentially P or vP
	1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	PBT profiler not available	Biowin 2 Biowin 3 Biowin 6	**0.48** **2.06** **0.003**	Potentially P or vP

*More degradation relevant information is generally warranted if Biowin 2 or 6 <0.5 and Biowin 3 is between 2.25 and 2.75

According to R.11 ECHA guidance on PBT assessment (ECHA, 2017a), a substance screens potentially P or vP, if Biowin 2 or 6 <0.5 and Biowin 3<2.25 (to 2.75).

All the trimer constituents screen 'potentially P/vP' as Biowin 2 and 6 is below 0.5 and Biowin 3 is below 2.25. For the dimers, Biowin 6 is below 0.5, but the Biowin 3 predictions are between 2.28 and 2.51, indicating that they are 'potentially P/vP' and that more degradation relevant information is generally warranted. The potential persistency of the dimers is supported by the PBT profiler predictions which predict the dimers to be very persistent in the sediment compartment. Currently there is no universally accepted definition of model domain for the Biowin models, however, the molecular weights are within the training set range for all the structures predicted. For the PBT profiler, there are likewise no definition of domain, but the predicted structures all fall within the indicated specifications and molecular weight range for the model.

3.1.2.1.2 Screening tests

Ready biodegradability tests have been carried out with OAPP and with two of its constituents.

Screening test with the registered substance

A ready biodegradability test with OAPP was conducted according to the Japanese equivalent to OECD TG 310 (Ready Biodegradability - CO2 in sealed vessels) with activated sewage sludge which is reported in the OAPP registration dossier. The test was conducted in sealed vessels in the dark at 20±1 °C. OAPP was dissolved in tetrahydrofuran and dispensed onto a filter paper where the solvent was allowed to evaporate to dryness. The filter papers were then added to the test vessels. The biodegradation of the test item was assessed at a concentration of 20 mg C/L by measuring the evolution of inorganic carbon present in the headspace of the vessel. The mean total organic carbon in the control vessels was 0.86 mg/L, the toxicity control reached 38% degradation after 14 days and the positive control (sodium benzoate) attained 83% degradation after 14 days. The test therefore fulfills the validity criteria of the OECD TG 310 and the reliability of the test is assessed as reliable without restrictions. After 28 days, the test item attained 4% degradation. Based on these results OAPP is not readily biodegradable.

It should be noted that ready biodegradability tests are not capable of discriminating between the relative degradation for each of the constituents. It is possible that the limited amount of biodegradation observed is associated with the less lipophilic constituents since these will have a smaller degree of sorption to organic matter and therefore will be more bioavailable to the microorganisms present in the test system. Some of the constituents

with very high log Kow e.g., dimers and trimers are likely to have a very limited bioavailability due to sorption and low water solubility.

Screening tests with constituents of the registered substance

A ready biodegradability test equivalent to OECD TG 301 C (modified MITI I) has been carried out with the monoalkylated phenol constituent 4-(*α,α*-dimethylbenzyl)phenol (EC 209-968-0, CAS 599-64-4) and is reported in the OAPP registration dossier. After 28 days, the test item showed 0 % degradation as measured by oxygen consumption and 7 % degradation as measured by HPLC analysis. In conclusion, the constituent is not readily biodegradable (NITE 2003a). As the report is written in Japanese it has not been possible to assign a reliability to the study.

A ready biodegradability test equivalent to OECD TG 301 C has been carried out with the dimer 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7) and reported in the registration dossier for EC 228-846-8[3]. The test was performed with the 100 mg/L of the test substance, inoculated with mixtures of unadapted micro-organisms in 30 mg/L inoculum at 25±1 °C for 28 days. The percentage degradation of the reference substance aniline showed 53 % after 7 days and 66% after 14 days. The oxygen uptake of the inoculum blank was less than 60 mg/O_2/l in 28 days and pH stayed stable at 7.2. The test substance remained undissolved and the degradation was calculated based on the BOD. After 28 days, the test item showed 0 % degradation as measured by oxygen consumption and 3 % degradation as measured by HPLC analysis. In conclusion, the dimer was not readily biodegradable (NITE 2002a). The reliability of the study is assessed as reliable with restriction.

The registration dossier for EC 228-846-8 contains a modified MITI (II) test (302C). The study used a mixed population of active sludge micro-organisms from 10 different UK sites. The test was conducted with 30 mg/L test substance in vessels with increased volume (500 ml glass bottles) with a temperature of 24-25 °C. The dossier reports 18% degradation based on mean oxygen consumption after 14 days and 64% after 28 days. Compound specific analysis showed a mean primary degradation of 82% after 28 days in deionised water. For both oxygen consumption and primary degradation, high variation was found within the replicates. No information on toxicity, lag phase or preadaptation is stated, and there is no outcome of the performed aniline test. It is therefore not possible to assess the validity of the test and the reliability of the test is not assignable. As the substance does not reach a level of 70% mineralisation (O2 uptake) within 14 days, the substance is potentially P or vP.

3.1.2.1.3 Simulation tests

3.1.2.1.3.1 Biodegradation in water

Based on Biowin predictions, the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) screens at the most stable dimer constituent, as seen in Table 6. 1,1,3-trimethyl-3-phenylindan ('the dimer') was therefore selected as worst-case constituent for the dimer fraction and have been tested in an OECD TG 309 (Aerobic Mineralisation in Surface Water – Simulation Biodegradation Test), as reported in the OAPP registration dossier.

The study was run with radioactive labelled [^{14}C]1,1,3-trimethyl-3-phenylindan over 60 days at two concentrations, 1 and 10 µg/L, at 12 °C. Water was collected from River Harbourne, Devon, UK and [^{14}C]Benzoic acid was used as positive control. The study achieved generally good recovery with limited degradation demonstrated during the study period (Table 7). The reference test with benzoic acid reached 77% degradation after 14 days in one vessel that was dosed twice and the duplicate vessel was omitted from any

[3] https://echa.europa.eu/registration-dossier/-/registered-dossier/12609

calculations due to a leak/non-dosing. The degradation of benzoic acid satisfied the validity criteria of the reference substance as described in OECD TG 309 and the study is assessed as reliable without restriction.

Table 7: Overview of degradation of 1,1,3-trimethyl-3-phenylindan in OECD TG 309

Day	1 µg/L		10 µg/L	
	% Applied radioactivity	% as [14C]1,1,3-trimethyl-3-phenylindan	% Applied radioactivity	% as [14C]1,1,3-trimethyl-3-phenylindan
0	113	99.74	99	99.74
7	92	91.02	94	90.09
14	91	89.59	91	80.36
28	104	91.81	101	88.80
42	106	95.78	103	82.74
60	104	90.11	98	75.94

Mineralisation was measured at five time points during the study (7, 14, 28, 42 and 60 days) and accounted for up to 11.2% and 10.6% for the 1 and 10 µg/L concentrations, respectively. Less than 1% was observed at day 7 at both concentrations. The peak mineralisation was reached at day 28 for the 1 µg/L study and at day 14 for the 10 µg/L study. Notably, in the sterile control, mineralisation also reached 5.7 % at day 60. Overall, a lower primary degradation was observed at the low concentration compared to the high concentration, which is not reflected by the mineralisation data where the two studies reached similar levels, although in the study with the high concentration, it was reached faster than at the low concentration.

In both studies, one main metabolite was identified, namely 1,3-dimethyl-3-phenyl-2,3-dihydro-1H-indene-1-carboxylic acid. In the study, a suggested degradation pathway to the carboxylic acid was elucidated as shown in Figure 1 below.

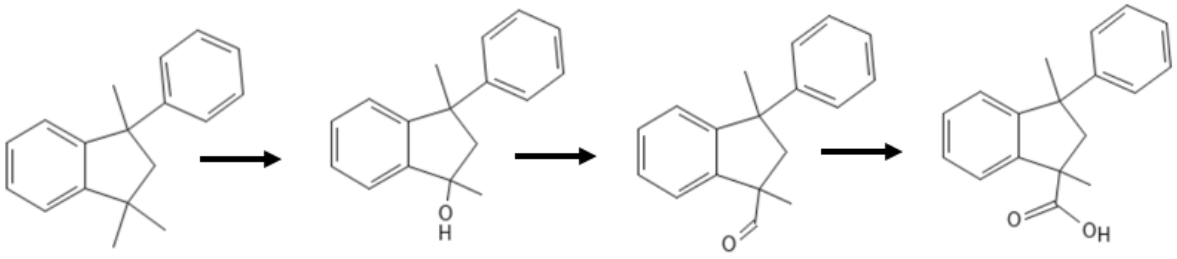


Figure 1: Suggested degradation pathway in the OECD TG 309. The pathway is initiated with a methyl group hydroxylation, which is further oxidised to a carboxylic acid

A kinetic evaluation of the degradation data was performed in CAKE v3.4. DegT50 and DegT90 values were calculated by Single First-Order (SFO), First-order Multiple Compartments (FOMC), Double-First-Order in Parallel (DFOP) and Hockey-Stick (HS) models. As only limited degradation was observed in the study, the bi-phasic models (FOMC, DFOP, HS) were more strained to make a fit and a visual assessment of the

goodness of fit, concluded that the SFO was the most appropriate. This is also supported by ECHA R.11 PBT guidance which state 'Use of bi-phasic kinetic models, fast initial decrease in test substance concentration followed by a slower decline, is recommended to cases where an acceptable single-first order (SFO) fitting is not possible' (ECHA, 2017a). Furthermore, the χ^2-test was used as a tool to compare the goodness of fit of the four models (SFO, FOMC, DFOP and HS) and the t-test was used to assess the reliability of the estimated rate parameters for each model (Table 8).

Notably, all models gave rise to high DegT50 values above the vP criteria (when taking k2 and overall values into account for HS and DFOP) as seen in Table 8. It is also important to note that the DegT50 values derived from the kinetic models were extrapolated beyond the experiment period of 60 days. The DegT50 was calculated to be 205-542 days using the SFO model. The degradation rate (k) parameter is considered significantly different from zero if the probability is smaller than 0.05. For this model, the degradation rate (k) does not differ significantly from zero (p>0.05) in the 1 µg/L study, meaning that the parameter is either very uncertain due to variability in the data or the model is not adequate with respect to the data.

Table 8: Kinetic evaluation of OECD TG 309 data in CAKE v3.4

Model	Concentration (µg/L)	DegT50 (days)	DegT90 (days)	χ2 error	Parameter	t-test
SFO	1	**542**	1800	4.68	k 0.0013	0.12
	10	**205**	681	4.37	k 0.003	0.027
FOMC	1	**>10 000**	>10 000	2	α 0.0044 β 1.82E-007	N/A N/A
	10	**1390**	>10 000	4.46	α 0.17 β 24.08	Nd* Nd*
HS	1	Overall: **>10 000** K1: 39.1 **K2: >10 000**	>10 000	2.16	k1 0.018 k2 1.55E-010	Nd* Nd*
	10	**Overall >10 000** **K1: 61.6** **K2: >10 000**	>10 000	4.83	k1 0.011 k2 5.87E-035	0.08 0.05
DFOP	1	Overall: **>10 000** K1: 0.95 **K2: >10 000**	>10 000	4.67	k1 0.734 k2 1.55E-015 g 0.081	0.48 0.5 N/A
	10	**Overall: 202** **K1: 202** **K2: 934**	672	5.49	k1 0.0034 k2 7.42E-004 g 1	0.49 0.5 N/A

*Note: Statistics may be missing because the covariance matrix could not be fully calculated. This usually means that there was insufficient data provided or the model setup was inappropriate.

According to the PBT guidance (ECHA, 2017a) and REACH Annex XIII, the criteria for persistent (P) and very persistent (vP) are fulfilled for a half-life in fresh water above 40 and 60 days, respectively. Based on the presented findings, the dimer is considered to fulfil the P/vP criteria of REACH Annex XIII.

Persistency read-across from dimer to trimer

According to REACH Annex XI, a read-across approach can be applied using substances whose physicochemical, toxicological and ecotoxicological properties are likely to be

similar to the substance in question or follow a regular pattern as a result of structural similarity. For persistency, all of these conditions are met in a read-across from the dimer 1,1,3-trimethyl-3-phenylindan (the source substance) to 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane that has been identified by registrants as a main trimer ('the trimer', the target).

Similarity in physico-chemical properties

No measured physico-chemical properties are available for the source or target substance but QSAR predictions are available, as reported in Table 4. Both substances are predicted to have low water solubility and high Log Kow and are thus expected to be lipophilic. The target trimer is more lipophilic than the dimer which is to be expected due to the additional 2-phenylpropyl fragment in its structure.

The source substance dimer 1,1,3-trimethyl-3-phenylindan has a predicted water solubility of 0.0339 mg/L, a vapour pressure of 0.0924 Pa (25 °C) and a Log Kow of 5.91.

The target substance trimer 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan has a predicted water solubility of 124.8 ng/L, a vapour pressure of 5.58*10-6 Pa (25 °C) and a Log Kow of 8.98.

Structural similarity

The main trimer can be described as the dimer with the addition of a 2-phenylpropyl fragment. Strikingly, the 2-phenylpropyl add-on to the dimer is on the same carbon where the dimer was shown to be the most susceptible to degradation in the OECD TG 309 study. Also of note, is the fact that no new functional groups are introduced in the trimer compared to the dimer, it is in essence more of the same. It can correspondingly be hypothesised that the trimer is at least as persistent as the dimer (Figure 2).

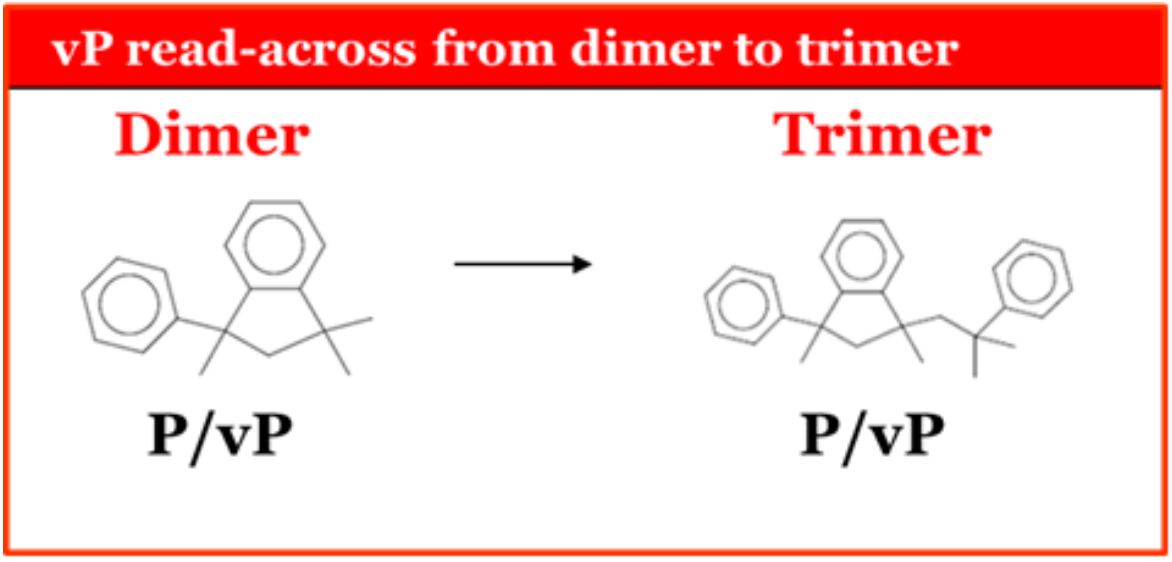


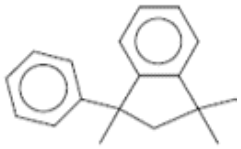
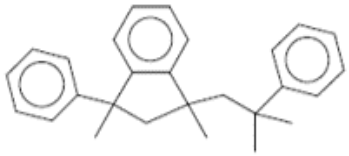
Figure 2: P/vP read-across from the dimer to the trimer

Computational evidence

No experimental data is available on any of the trimers. To assess the validity of the read-

across hypothesis that the trimer fulfils the P/vP criteria, the dimer and trimer can be compared computationally. Table 9 shows the increasing trend in predicted persistency from the dimer to the trimer.

Table 9: Biowin, BioHCwin (US EPA, 2023) and CATALOGIC (OASIS LMC, 2022) predictions for the dimer and trimer

Model	**Dimer 1,1,3-trimethyl-3-phenylindan**	**Trimer 1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan**
Structure		
Experimental data	**DegT50: 205-542 days**	**No experimental data**
Biowin 1 (lower number indicate slower degradation)	**0.40**	**0.28**
	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Biowin 2 (lower number indicate slower degradation)	**0.12**	**0.027**
	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Biowin 3 (lower number indicate slower degradation)	**2.27**	**1.82**
	Weeks to months	Months
Biowin 4 (lower number indicate slower degradation)	**3.20**	**2.89**
	Weeks	Weeks
Biowin 5 (lower number indicate slower degradation)	**0.24**	**0.046**
	Not Ready Degradable	Not Ready Degradable
Biowin 6 (lower number indicate slower degradation)	**0.11**	**0.001**
	Not Ready Degradable	Not Ready Degradable
Biowin 7 (lower number indicate slower degradation)	**-0.83**	**-1.48**
	Does Not Biodegrade Fast	Does Not Biodegrade Fast
BioHCwin (Half-life)	**20 days**	**116 days**
CATALOGIC Primary Half Life	**3m 10 days**	**2m 16 days**
CATALOGIC Ultimate Half Life	**6y 5m 7 days**	**7y 4m 20 days**

Biowin predictions

For Biowin, all of the models show a trend towards slower degradation going from the dimer to the trimer. Regarding the reliability of the predictions, the molecular weights are all within the training set range for all the structures predicted. As explained, the trimer is structurally composed of the dimer connected to an additional monomer, linked through a CH2 fragment. Searching for a CH2 fragment attached to quaternary carbons (as in the trimer) in the training set of the ultimate and primary Biowin models (Biowin 3 and 4), returns three relevant structures which also contain this fragment demonstrating that the Biowin models are familiar with the degradation potential of this type of fragment. For the three structures, the experimental values in the training set data are in proximity with their predictions and are also within range of the values for the trimer as seen in Table 10. For all four substances, the presence of the quaternary carbon is the most influential fragment in the Biowin predictions. In Biowin 3 and 4, this fragment has a negative coefficient and the presence of such a quaternary carbon therefore slows down the rate of degradation in the Biowin predictions.

Table 10: Biowin 3 and 4 scores for structures with a CH2 fragment attached to quaternary carbons in the Biowin 3 and 4 training set.

	Biowin3_Obs	Biowin4_Obs	Biowin3_Pred	Biowin4_Pred
benzethonium chloride	1.88	3.08	1.74	2.98
nonane, 2,2,4,4,6,8,8-heptamethyl	1.68	2.43	2.06	3.06
fraction of Triton X-100	2.21	3.21	1.80	3.02
1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan	-	-	1.82	2.89

The fragments in the dimer and trimer are all fully covered in the Biowin and BioHCwin models. However, the trimer has three occurrences of quaternary carbons while in the training set for Biowin 7, the maximum number of occurrences is two. The trimer also has three bonds from an aromatic ring to a carbon and for the BioHCwin model this is not fully represented in the training set. The extra occurrences of quaternary carbons and aromatic ring carbon bonds in the trimer over the dimer, however, are expected to add to its persistency, or at least, not make the trimer less persistent than the dimer.

The BioHCwin is a model that includes several new fragments from petroleum hydrocarbons, while maintaining the original basic MITI fragments. The half-life for the dimer is notably low compared to the experimental value, however according to the ECHA R7b guidance, BioHCwin is known to underestimate the half-life for branched compounds. Furthermore, due to the training set containing compounds tested with co-exposure leading to potential co-metabolism, this may also lead the model to underestimate the degradation half-life. BioHCwin should accordingly not be used to support a conclusion of not P/vP (ECHA, 2017b). The trimer is, however, predicted to be far above the P/vP criteria in this model, which supports the vP read-across.

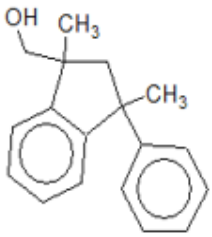
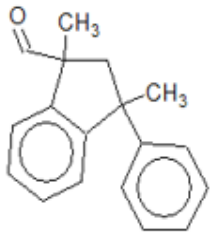
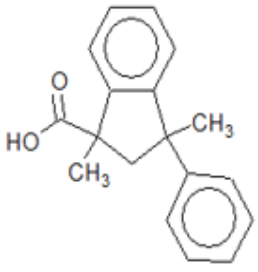
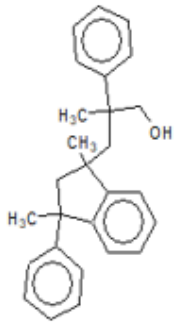
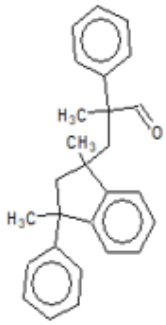
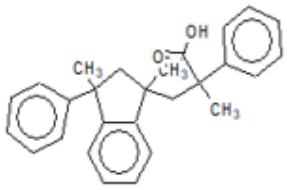
CATALOGIC predictions

Further computational analysis of the degradation of the dimer and trimer have been performed in the CATALOGIC 301 C model. As seen in Table 9, CATALOGIC predicts both primary and ultimate half-lives to be above the P/vP criteria for both the dimer and trimer. Similarly to BioHCwin, CATALOGIC underestimates the primary half-life of the dimer compared to the experimental value, i.e. the half-life is predicted to be a factor 2-5 shorter than found experimentally. A similar level of underestimation of the half-lives could be expected for the trimer. CATALOGIC predicts the ultimate half-life to be longer for the trimer (>seven years) compared to the dimer (>six years), however, CATALOGIC also predict the primary half-life of the trimer to be shorter than the half-life of the dimer. When looking at the degradation maps (301C v13.18 / CATALOGIC v5.16.1.10) there are two transformation reactions for the dimer and trimer at the first level: methyl group oxidation and aromatic ring hydroxylation. Methyl group oxidation is there once for both the dimer and the trimer, but the aromatic ring hydroxylation is counted 7 times for the trimer and only five times for the dimer as there are fewer positions for the same reaction to take place. This leads to a lower parent quantity for the trimer, and consequently a shorter primary half-life.

However, in the experimental study, hydroxylation of the aromatic ring was not observed. As the degradation of the dimer was shown to be driven by the methyl group hydroxylation, the primary half-life of both constituents is similarly expected to be driven by the methyl group hydroxylation. The CATALOGIC rule used to predict the methyl group hydroxylation targets only structures with two methyl groups connected via a single carbon – and in both the dimer and trimer this fragment occurs only once. Other methyl group oxidations are also predicted in CATALOGIC, however they are ranked lower in the hierarchical application of transformation reactions, after the aromatic ring hydroxylation.

As seen in Table 11, CATALOGIC predicts a lower overall probability of the methyl group hydroxylation occurring for the trimer compared to the dimer, which would give rise to a slower half-life for the trimer compared to the dimer. In line with the OECD TG 309 study, the methyl group hydroxylation is the most probable predicted degradation pathway for both the dimer and trimer.

Table 11: Most probable predicted degradation pathway in CATALOGIC for the dimer and trimer. P=Overall probability

1,1,3-trimethyl-3-phenylindan (DIMER)	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan (TRIMER)
P=0.0341 631. Methyl group hydroxylation  P=0.0341 107. Primary hydroxyl group oxidation  P=0.0341 76. Aldehyde oxidation  P=0.00124 635. Methyl group hydroxylation	P=0.0331 631. Methyl group hydroxylation  P=0.0331 107. Primary hydroxyl group oxidation  P=0.0331 76. Aldehyde oxidation  P=0.00122 632. Methyl group hydroxylation

CATALOGIC uses OECD TG 301C training data as well as rule-based information to predict

degradation kinetics and pathways, and correspondingly has multiple domains. The dimer and trimer are within the parametric and mechanistic domain, but both are outside the structural domain of the model, since 37.5 and 25%, respectively, of the fragments are unknown to the model. In more detail, the same three atom centred fragments (ACFs) are unknown to the model, shown below for the trimer in Figure 3.

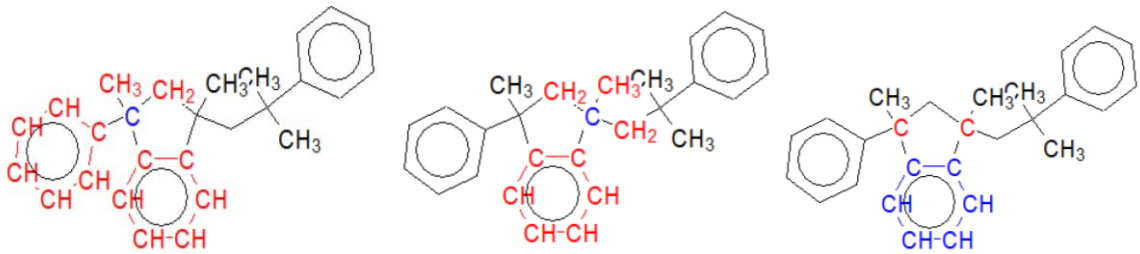


Figure 3: The three unknown atom centred fragments in both the dimer and trimer, indicated in red (center of fragment in blue).

The common feature of these fragments is the presence of a quaternary carbon in combination with one or more aromatic rings, not known by the model. As discussed above, the presence of quaternary carbons are expected to add to the stability of the structure. Furthermore, as these fragments have already been tested experimentally in the OECD TG 309 study with the dimer, it can be inferred that they do not lead to a potentially faster, unidentified pathway not covered by the model – on the contrary, the model underestimates the primary half-life for the dimer by a factor of around 2-5 compared to the experimental value, which supports that the uncertainty in the predictions do not exaggerate the persistency.

Additionally, as discussed above, if degradation occurs, the most likely predicted degradation pathway for the dimer is a methyl group hydroxylation and oxidation leading to the formation of a carboxylic acid on the same carbon that was susceptible to degradation in the OECD TG 309 study, which also identified this carboxylic acid as the main metabolite (Figure 1). As mentioned above, the other methyl groups on the dimer and trimer are not as available for hydroxylation, and as the predicted pathways in CATALOGIC are confirmed experimentally for the dimers in the OECD TG 309 study, it can be concluded that the structures and their fragments are represented well in the CATALOGIC model.

Considering all the evidence above, the (Q)SAR predictions are considered acceptable for the purpose of supporting the read-across hypothesis that the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane) (EC 255-584-1, CAS 41906-71-2) is at least as persistent as the dimer (1,1,3-trimethyl-3-phenylindan) (EC 223-467-4, CAS 3910-35-8).

The trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindane) (EC 255-584-1, CAS 41906-71-2) is accordingly considered to fulfil the criteria for P/vP (degradation half-life in water >60 days) of REACH Annex XIII.

Full reports (QPRFs) on the CATALOGIC predictions can be seen in Annex 1, available as a separate document.

3.1.2.1.3.2 Biodegradation in sediment

No data has been identified for the dimers or trimers.
3.1.2.2 Biodegradation in soil

3.1.2.2.1 Simulation tests in soil

No data has been identified for the dimers or trimers.

3.1.3 Field data

No information has been identified for the dimers or trimers.

3.1.4 Summary and discussion of degradation

Simulation testing on the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8), shows that the dimer fulfils the P/vP criteria of REACH Annex XIII. This dimer was chosen as a potential worst-case representative for the dimer fraction to clarify the P/vP for the group.

No experimental data is available for the trimers. However, based on a read-across from the dimer (1,1,3-trimethyl-3-phenylindan) (EC 223-467-4, CAS 3910-35-8) to the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2), the trimer (EC 255-584-1, CAS 41906-71-2) can also be considered to fulfil the P/vP criteria of REACH Annex XIII (degradation half-life in water >60 days).

3.2 Environmental distribution

3.2.1 Adsorption/desorption

No experimentally derived K_d values for individual constituents of OAPP have been identified in the registration dossiers or in the literature.

K_{oc} values for the dimers and trimers have been estimated in KOCWIN v2.00 by two different estimation methods (Kow and MCI, (US EPA, 2023)). According to these estimates the constituents have strong adsorptive properties and are expected to be immobile in soil (based on classification of a substance's mobility in soil according to McCall et al., 1980). For these models there are no universally accepted definition of model domain. The dimers and trimer are within the molecular weight range of the training set for KOCWIN v2.00.

Table 12: Estimated log Koc values for the dimers and trimers

Group	Substance	Estimated Log Koc values
Dimers	1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	Kow method: 5.13 MCI method: 5.05
	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	Kow method: 5.65 MCI method: 5.08
	1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	Kow method: 5.58 MCI method: 5.08
Trimers	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-	Kow method: 7.79

Group	Substance	Estimated Log Koc values
	phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	MCI method: 7.30
	1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	Kow method: 8.24 MCI method: 7.32
	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	Kow method: 8.19 MCI method: 7.34
	1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	Kow method: 8.24 MCI method: 7.32

3.2.2 Volatilisation

No information on volatilisation is available in the registration dossiers and no information has been identified in the literature for the substance or for its individual constituents. Henry's law constants have been estimated for the dimers and trimers in HENRYWIN v3.20 in EPIsuite (US EPA, 2023), using the Bond method. The Henry's law constants for the dimers and the trimers indicate a low potential for volatilisation. For this model there is no universally accepted definition of model domain. The dimers and trimer are within the molecular weight range of the training set used for developing the Bond method.

Table 13: Predicted Henry's law constant for the dimers and trimers

Group	Substance	Henry's law constant (atm*m3*mol-1)
Dimers	1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	$7.3*10^{-4}$
	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	$8.2*10^{-4}$
	1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	$9.7*10^{-4}$
Trimers	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	$1.37*10^{-4}$
	1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	$1.82*10^{-4}$
	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	$1.65*10^{-4}$
	1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	$1.82*10^{-4}$

3.2.3 Distribution modelling

Fugacity level III modelling (EPIweb) was performed for dimers and trimers for two

scenarios:

1. Assuming equal and continuous emissions to water, soil and air
2. Assuming 100% emission to water

According to these modelling results, the constituents are expected to distribute primarily to soil and sediment if released equally and continuously to water, soil and air. If released only to water, the constituents are expected to distribute primarily to sediment.

Table 14: Predicted environmental distribution for the dimers and trimers

Group	Substance	Emission	Distribution to water (%)	Distribution to soil (%)	Distribution to sediment (%)	Distribution to air (%)
Dimers	1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	Water, soil & Air	6	60	33	<1
		Water	15	0	84	<1
	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	Water, soil & Air	6	61	33	<1
		Water	16	0	84	0
	1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	Water, soil & Air	6	61	33	<1
		Water	16	0	84	0
Trimers	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	Water, soil & Air	3	40	57	<1
		Water	5	0	95	0
	1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	Water, soil & Air	5	48	47	0
		Water	10	<1	90	0
	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	Water, soil & Air	4.5	49	46	<1
		Water	9	0	91	0
	1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	Water, soil & Air	5	48	47	0
		Water	10	<1	90	0

3.2.4 Field data

No information has been identified for the dimers or trimers.

3.2.5 Summary and discussion of environmental distribution

The dimers and trimers have strong adsorptive properties and are expected to be virtually immobile in soil. When released to the environment, they will tend to distribute primarily to soil and/or sediment depending on the release profile.

3.3 Data indicating potential for long-range transport

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (e) REACH.

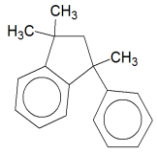
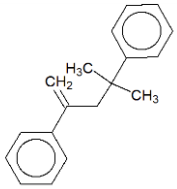
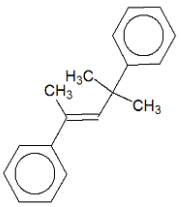
3.4 Bioaccumulation

3.4.1 Bioaccumulation in aquatic organisms (pelagic & sediment organisms)

Dimers

As shown in Table 4, the dimers have estimated log Kow values of 5.9 to 6.4, which exceed the screening criteria for B/vB (log Kow >4.5; ECHA, 2017a). Table 15 gives an overview of estimated BCF and BAF values for the dimers based on the BCFBAF regression model and the Arnot Gobas BCF/BAF models (upper trophic level, including biotransformation) in BCFBAF v3.01. The dimers are within the applicability domain of the Arnot Gobas and the BCFBAF models and the predictions indicate that the dimers are potentially B or vB. No suitable structural analogs with testing data for bioaccumulation could be identified in the OECD (Q)SAR Application Toolbox.

Table 15: Overview of QSAR predictions for the dimers

Constituent	Structure	(Q)SAR	Conclusion
1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8		BCFBAF, BCF: 3681 Arnot Gobas, BCF: 2482 Arnot Gobas, BAF: 7388 kM = 0.0894 /day (10 g fish)	Potentially B or vB
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7		BCFBAF, BCF: 9201 Arnot Gobas, BCF: 1711 Arnot Gobas, BAF: 13730 kM = 0.0927 / day (10 g fish)	Potentially B or vB
1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7		BCFBAF, BCF: 8165 Arnot Gobas, BCF: 2241 Arnot Gobas, BAF: 21760 kM = 0.0740 / day (10 g fish)	Potentially B or vB

A bioaccumulation study performed according to the equivalent protocol of OECD TG 305

was carried out under the existing chemicals survey conducted by the Japanese Government (NITE 2002b). In this study, carp (*Cyprinus carpio*) were exposed for 60 days to two different concentrations of 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7). The test organisms (8±4 cm) were exposed to concentrations of 10 µg/L and 1 µg/L at 24±2 °C with flow-through conditions for 60 days and depurated for 16 days. The concentration of dissolved oxygen was ≥ 60% saturation. The stock population of fish was acclimated for at least two weeks (mortality <5% in 7 days). The concentrations of the test substance was maintained within ± 20% of the mean of the measured values during the uptake phase. No abnormality nor mortality was observed during the study. The lipid content of the fish was measured at the beginning and at the end of the uptake and end of the depuration phase. Analytical measurements of the test substance in fish and test media were performed once a week with GS/MS (recoveries 95.8-108.3%, limit of detection 0.05 µg/L). The study is assessed as reliable with restriction.

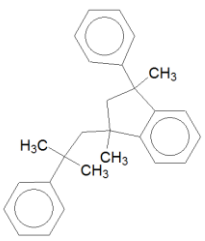
The study did not reach steady state as the average BCF values varied more than 20 % over the 3 consequent measurements and therefore the BCF_{SS} was not calculated. BCF values were calculated as the ratio of concentration in the fish and in the water, measured throughout the uptake phase, which gave rise to BCF values of 427-3330 for the high exposure group (10 µg/L) and 423-4410 for the low exposure group (1 µg/L). The study also reports BCF values normalised to 4% lipid content, which recalculated to 5% lipid content gives BCF_L values of 368-5208 (10 µg/l) and 404-4691 (1 µg/L). There is no reliable approach to correct such BCF values for growth dilution as stated in the OECD TG 305 and discussed by Crookes & Brooke (2011), therefore no growth corrections have been applied.

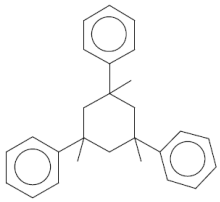
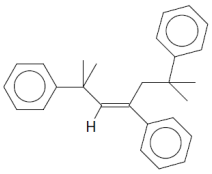
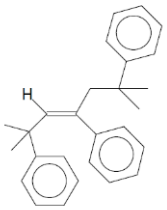
Trimers

As shown in Table 4, the trimers have estimated log Kow values of 9.0 to 9.5 which exceed the screening criteria for B/vB (log Kow >4.5; ECHA, 2017a).

Table 16 gives an overview of estimated BCF and BAF values for the trimers based on the BCFBAF regression model and the Arnot Gobas BCF/BAF models (upper trophic level, including biotransformation) in BCFBAF v3.01. The trimers are within the applicability domain of the Arnot-Gobas and the BCFBAF models. Due to the hydrophobic nature of the constituents, uptake through the food may exceed uptake over the gills so the BCF predictions are not considered to be relevant and are given a low weight compared to the bioaccumulation estimates. The Arnot-Gobas BAF estimate is 15810-177800 for the trimers (upper trophic level, including biotransformation rate estimates) thus indicating a high potential for bioaccumulation. No suitable structural analogs with testing data for bioaccumulation could be identified in the OECD (Q)SAR Application Toolbox. The predictions indicate that the trimers are potentially B or vB.

Table 16: Overview of QSAR predictions for the trimers

Constituent	Structure	(Q)SAR	Conclusion
1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2		BCFBAF, BCF: 1426 Arnot Gobas, BCF: 113 Arnot Gobas, BAF: 177800 kM = 0.0109 / day (10 g fish)	Potentially B or vB

Constituent	Structure	(Q)SAR	Conclusion
1,3,5-triphenyl-1,3,5-trimethylcyclohexane		BCFBAF, BCF: 849 Arnot Gobas, BCF: 21 Arnot Gobas, BAF: 15810 kM = 0.004/ day (10 g fish)	Potentially B or vB
1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene		BCFBAF, BCF: 789 Arnot Gobas, BCF: 41 Arnot Gobas, BAF: 76540 kM =0.0016 / day (10 g fish)	Potentially B or vB
1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3		BCFBAF, BCF: 789 Arnot Gobas, BCF: 41 Arnot Gobas, BAF: 76540 kM =0.0016 / day (10 g fish	Potentially B or vB

OECD TG 305

A dietary OECD TG 305 (Bioaccumulation in Fish: Aqueous and Dietary Exposure) combined with elements from OECD TG 229 (Fish Short Term Reproduction Assay) for vitellogenin measurements, has been performed in 2017 with OAPP in Fathead minnow (*Pimephales promelas*). It was conducted in a flow-through setup with 14 days of uptake and 28 days of depuration. Five fish were sampled on uptake phase days 0, 7, 14 and depuration days 1, 2, 5, 8, 15, 21 and 28. Three samples of the food were taken on day 1, 7 and 14 of the uptake and day 4 on depuration and analysed. No information on the homogeneity of the substance in the spiked food is reported in the study. The concentration in the food was 250 µg/g (recovery 81-108%) for the reference substance hexachlorobenzene (HCB), 100 µg/g (recovery 99-105%) for 17β—estradiol, 0.39 mg/g (recovery 81-83%) for the dimers and 0.23 mg/g (recovery 90-107%) for the trimers.

At three points during the study the temperature was below 21±2°C (hourly measurements), which is not considered to have an impact on the integrity of the study. The concentration of dissolved oxygen was stable between 80-100%. In the test and control group no significant mortality or non-lethal effects were observed (cumulative mortality of 0.6% after 42 days). A reference test with HCB, one of the original twelve POPs, and 17β—estradiol however did give rise to mortality (cumulative mortality of 18.2% between day 10 and 42). Additionally, some fish experienced internal bleeding during the uptake phase. As a reference test is not a requirement in OECD TG 305, the main study is still considered valid as it fulfils the criteria in OECD TG 305. The study is considered reliable without restriction.

Table 17: Key results from the dietary bioaccumulation study (reported in the study report)

Parameter	Dimers	Trimers	HCB (reference substance)
Assimilation efficiency, α	**0.270**	**0.104**	**0.913**
k2, d^{-1} (depuration, growth-corrected)	**0.130**	**0.027**	**0.060**
Growth-corrected half-life (days)	**5.3**	**25.8**	**11.6**
BMFkg (growth corrected BMF)[1]	**0.0415**	**0.0775**	**0.307**
BMFkgL (growth and lipid corrected BMF)[2]	**0.0737**	**0.137**	**0.544**

[1]Reported as BMF in the study report but confirmed as BMFkg using the equations A7.5 and A7.9 in OECD TG 305 Annex 7
[2]Reported as BMFLipid in the study report but confirmed as BMFkgL using the equations A7.5 and A7.9 in OECD TG 305 Annex 7

During the study, growth rates of 0.0073 and 0.0045 was observed for the control and test group, respectively. Analytical monitoring was performed for the three dimers and seven potential trimer constituents were monitored, including 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2). The study compiled the raw data for the dimers and trimers into values for each group, therefore no recalculation can be made for the individual constituent. As shown in Table 17, uptake of both the dimers and trimers was observed in the study with depuration half-lives of 5.3 and 25.8 days, respectively. HCB had a depuration half-live of 11.6 days. The OECD validation ring test of dietary exposure in the OECD TG 305 in rainbow trout (*Oncorhynchus mykiss*), reported the growth-corrected depuration rate constants for HCB as 0.035±0.005 and 0.016±0.006 d^{-1}, with a feeding rate of 1.5% and 3% respectively (OECD, 2013). This corresponds to a mean depuration half-live of 19.8 and 43.3 days, respectively. The feeding rate in the present study was 2% and it is not clear whether the faster observed depuration of HCB is due to the observed toxicity, the combination with 17β—estradiol or caused by species differences. Growth and lipid-adjusted biomagnification factors of 0.073, 0.137 and 0.544 were obtained for the dimers, trimers and HCB, respectively. An estimation of corresponding kinetic BCF values can be performed in various ways by estimating the rate of uptake as stated in OECD TG 305 (overview of these approaches can be found in Crookes & Brooke (2011) and in the OECD TG 305 OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation (OECD, 2017). Based on these approaches, an OECD Dietary BCF Estimation Tool has been developed to estimate BCF values for dietary bioaccumulation studies which has been used to calculate BCF values for the dimer and trimer constituents (Table 18).

The different prediction methods have an indicative applicability domain as stated in the OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation (OECD, 2017). Method 3 (Inoue et al. 2012) was developed for carp and therefore cannot be used for this study on Fathead minnow. Method 1 has an indicative log Kow domain approximately from 3.5 to 8.3 and Method 2 has an indicative log Kow domain approximately from 3 to 8.2. The dimers are all within this range, however the trimers are just above, which add some level of uncertainty to the predictions. However, for the trimers, most of the predictions estimate BCF values exceeding 10 000, clearly above the vB criteria of 5000 according to REACH Annex XIII. This is most likely due to the very slow experimental depuration rate. The trimers consequently also have a long half-life of 25.8 which is more than double that of the reference POP substance (HCB at 11.6 days). As noted there is some uncertainty associated with this reference test, however the trimers also have a slower depuration than the mean HCB depuration (half-life of 19.8 days) observed in the OECD validation ring test with the lower feeding rate in line with the OECD TG 305 requirements. Most of the estimated BCF values for the dimer constituents are above 2000, which indicate that the dimers fulfil the B criteria according to REACH Annex XIII.

Table 18: Derived BCF values for the dimers and trimers using the OECD Dietary BCF Estimation Tool. Yellow indicates values >2000 (B) and red indicates values >5000 (vB).

Study input	Value
Mean weight at test start (g)	2.31
Uptake phase duration (days)	14
Growth rate, K_g (day^{-1})	0.0045
Mean fish lipid uptake end or depuration start (fraction)	0.097
Mean fish lipid depuration end (fraction)	0.061
Depuration phase duration (days)	28

	Dimers			**Trimers**			
	1,1,3-trimethyl-3-phenylindan	1,1' -(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene	1,1' -(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene	1,1',1''-[(3Z)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	1,1',1''-[(3E)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	1,3,5-triphenyl-1,3,5-trimethylcyclohexane	1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan
Substance Input							
Log kow	5.91	6.2	6.43	9.5	9.5	9.44	8.98
K_{2g}	0.1301			0.0269			
BMFgL	0.737			0.1374			
Method 1 BCF estimations							
Hayton and Barron (1990)	2076.0			10040.6			
Erickson and McKim (1990a)	2864.7			13854.7			
Barber et al. (1991)	2838.6			13728.5			
Barber (2003) - observed	1832.5			8862.8			
Barber (2001)	2941.9			14228.4			
Streit and Sire (1993)	556.9			2693.5			
Erickson and McKim (1990b)	2285.0			11051.4			
Sijm et al. (1995)	1929.7			9333.0			
Barber (2003) - calibrated	2313.6	2313.8		11191.2			
Tolls and Sijm (1995)	3981.9	4319.8	4608.1	52794.7	51912.3	45619.5	
Spacie and Hamelink (1982)	3434.3	3788.5	4095.2	55987.4	54861.9	46951.6	
Hendriks et al. (2001)	499.4	502.0	503.2	2441.4			
Thomann (1989)	778.4	613.9	471.1	66.5	71.2	121.0	
Method 2 BCF estimations							
Brookes and Crooke (2012)	1710.4			11737.7			

3.4.2 Bioaccumulation in terrestrial organisms (soil dwelling organisms, vertebrates)

No test data has been identified for the dimers or trimers.

3.4.3 Field data

No test data has been identified for the dimers or trimers.

3.4.4 Summary and discussion of bioaccumulation

The dimers have estimated log Kow values of 5.9 to 6.4 and the trimers have estimated log Kow values of 9.0 to 9.5 which all exceed the screening criteria for B/vB (Log Kow > 4.5; ECHA, 2017a). An overview of the bioaccumulative data for the dimers and trimers is presented below in Table 19.

Table 19: Summary of bioaccumulation data

Constituent	QSAR	Test data
Dimers		
1,1,3-trimethyl-3-phenylindan EC no.: 223-467-4 CAS no: 3910-35-8	BCFBAF, BCF **3681** Arnot Gobas, BCF **2482** Arnot Gobas, BAF **7388** Log kow 5.91	**BCF 499-3982** **most above 2000** (OECD 305, Fathead minnow)
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene EC no.: 228-846-8 CAS no.: 6362-80-7	BCFBAF, BCF **9201** Arnot Gobas, BCF 1711 Arnot Gobas, BAF **13730** Log kow 6.2 (measured)	**BCF 368-5208** (OECD 305, carp) **BCF 502-4320** **most above 2000** (OECD 305, Fathead minnow)
1,1'-(1,3,3-trimethylprop-1-ene-1,3-diyl)dibenzene EC no.: 228-396-2 CAS no.: 6258-73-7	BCFBAF, BCF **8165** Arnot Gobas, BCF **2241** Arnot Gobas, BAF **21760** Log kow 6.43	**BCF 503-4608** **most above 2000** (OECD 305, Fathead minnow)
Trimers		
1,3-dimethyl-1-(2-methyl-2-phenylpropyl)-3-phenylindan EC no.: 255-584-1 CAS no.: 41906-71-2	Arnot Gobas, BAF **177800** Log kow 8.98	**BCF 121-46 952** **Most above 10 000** (OECD 305, Fathead minnow)
1,3,5-triphenyl-1,3,5-trimethylcyclohexane	Arnot Gobas, BAF **15810** Log kow 9.44	**BCF 71-54 862** **Most above 10 000** (OECD 305, Fathead minnow)
1,1',1''-[(3*E*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene	Arnot Gobas, BAF **76540** Log kow 9.5	**BCF 67-55 987** **Most above 10 000** (OECD 305, Fathead minnow)
1,1',1''-[(3*Z*)-2,6-dimethylhept-3-ene-2,4,6-triyl]tribenzene CAS no.: 957070-06-3	Arnot Gobas, BAF **76540** Log kow 9.5	**BCF 67-55 987** **Most above 10 000** (OECD 305, Fathead minnow)

For the dimers, BCF predictions within the applicability domain of the models are in the range 1711-2482. The Arnot-Gobas BAF estimate is 7388-21760 (upper trophic level, including biotransformation rate estimates). The QSARs predictions indicate that the dimers are potentially B or vB.

A bioaccumulation study OECD TG 305 (reliable with restrictions) performed with the dimer 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7) in carp (*Cyprinus carpio*) gave a BCF_L in the range of 368—5208 for the high exposure group (10 µg/L) and 404—4691 for the low exposure group (1 µg/L). A reliable without restriction dietary OECD TG 305 fish bioaccumulation study performed with OAPP in Fathead minnow (*Pimephales promelas*) gave a depuration half-life of 5.3 days for the dimers and a growth and lipid-adjusted biomagnification factor of 0.073. The estimated corresponding BCF values is in the range 499—4608 depending on the estimation method (most are above 2000). The dimers have shown a potential to reach high levels in fish, both in carp and in the fathead minnow where the BCF values are above the B criteria (BCF >2000) of REACH Annex XIII. This accumulation is furthermore supported by the (Q)SAR predictions.

For the trimers, BCF predictions using two (Q)SAR models for which the trimers fall within the applicability domain are: 21—113 (Arnot-Gobas, upper trophic level, including biotransformation), 789—1426 (BCFBAF). Due to the hydrophobic nature of the constituent, uptake through the food may exceed uptake over the gills so the BCF predictions are not considered to be relevant and are given a low weight compared to the bioaccumulation estimates. The Arnot-Gobas BAF estimate for the trimers is 15 810—177 000 (upper trophic level, including biotransformation rate estimates) thus indicating a high potential for bioaccumulation. The trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) concluded to be very persistent in water, is predicted to be the most bioaccumulative of the trimers.

A reliable without restriction dietary OECD TG 305 fish bioaccumulation study performed with OAPP in Fathead minnow (*Pimephales promelas*) gave a depuration half-life of 25.8 days for the trimers and a growth and lipid-adjusted biomagnification factor of 0.137. The estimated corresponding BCF value of the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is in the range of 121-46 952depending on the estimation method (most are above 10 000). 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is therefore considered to fulfil the vB criteria (BCF > 5000) according to REACH Annex XIII.

3.5 Summary and discussion of environmental fate properties

The dimers and trimers have strong adsorptive properties and are predicted to distribute primarily to sediments and soil, where they can be considered immobile.

Simulation testing on the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8), shows that it fulfils the P/vP criteria of REACH Annex XIII (degradation half-life in water >60 days). This dimer was chosen as a potential worst-case representative for the dimer fraction to clarify the P/vP for the group. No experimental data is available for the trimers; however, based on read-across from 1,1,3-trimethyl-3-phenylindan, the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) can also be considered to fulfil the P/vP criteria of REACH Annex XIII (degradation half-life in water >60 days).

The trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is considered to fulfil the vB-criterion of BCF>5000 in accordance with REACH Annex XIII.

4. Human health hazard assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (e) REACH.

5. Environmental hazard assessment

No chronic studies on aquatic organisms are available for the dimers or trimers. Only acute studies are available which do not provide useful results for highly lipophilic substances. This information is furthermore considered to be not relevant for the identification of the substance as SVHC in accordance with Article 57 (e).

6. Conclusions on the SVHC Properties

6.1 CMR assessment

Not relevant for the identification of the substance as SVHC in accordance with Article (e) of the REACH Regulation.

6.2 PBT and vPvB assessment

6.2.1 Assessment of PBT/vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance as vPvB. All available information, such as the results of standard tests, monitoring and modelling, information from the application of analogue approach (read-across) and (Q)SAR results, was considered together in a weight-of-evidence approach.

6.2.1.1 Persistence

Very limited biodegradation (4% after 28 days) was observed in an OECD TG 310 ready biodegradation study (reliable without restriction) with the whole substance OAPP. Ready biodegradation tests are not capable of discriminating between the relative degradation of each of the constituents and it is hypothesised that strong sorption of some of the extremely lipophilic constituents may reduce the bioavailability to degrading microorganisms. A ready biodegradability test equivalent to OECD TG 301 C (reliable with restrictions) carried out with the dimer of 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7) indicates that the constituent screens as potentially P or vP (0-3% biodegradation after 28 days).

Reliable QSAR predictions for biodegradation (Biowin 2, Biowin 3 and Biowin 6) indicate that all dimers screen as potentially P or vP but more degradation relevant information is generally warranted. As regards the trimers, reliable QSAR predictions for biodegradation using Biowin 2, Biowin 3 and Biowin 6 indicate that all the trimer constituents screen as potentially P or vP.

A reliable without restriction OECD TG 309 test (Aerobic Mineralisation in Surface Water –

Simulation Biodegradation Test) was performed on the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4; CAS 3910-35-8) which was chosen as a potential worst-case representative for the dimer fraction. [^{14}C] radiolabelled test material was used and the study conducted over 60 days at two concentrations, 1 and 10 µg/L, at 12 °C. After 60 days, 11.2% and 10.6% mineralisation was reached for the 1 and 10 µg/L concentrations, respectively. One main metabolite was identified in both experiments, 1,3-dimethyl-3-phenyl-2,3-dihydro-1H-indene-1-carboxylic acid. The study indicates that the dimer 1,1,3-trimethyl-3-phenylindan fulfils the P/vP criteria with a half-life in freshwater ≥205 days.

No experimental data is available for the trimers, therefore a read-across approach was used based on the structural similarity between the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) supported with (Q)SAR results in a weight-of-evidence approach. Based on a read-across approach with the dimer, it can be reasonably assumed that the trimer is at least as persistent as the dimer and thus the degradation half-life in water of the trimer exceeds 60 days. As a consequence, it is concluded that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) is very persistent in water (degradation half-life >60 days) in accordance with REACH Annex XIII.

Since OAPP contains the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2) with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets both the 'persistence' (P) (degradation half-life in water > 40 days) and 'very persistent' (vP) (degradation half-life in water > 60 days) criteria in accordance with Annex XIII, points 1.1.1 (b) and 1.2.1 (a), of the REACH Regulation.

6.2.1.2 Bioaccumulation

The dimers and trimers both screen as potentially B and vB with log kow values > 4.5 based on QSAR estimates.

The dimers have shown a potential to reach high levels in fish, both in carp (aqueous OECD TG 305 study performed on CAS 6362-80-7; reliable with restrictions) and in the fathead minnow (dietary OECD TG 305 study performed on the whole substance; reliable without restrictions) where the BCF values ranged from 499—4608 depending on the estimation method (most above 2000). This accumulation is furthermore supported by (Q)SAR predictions.

As regards the trimers, the dietary OECD TG 305 (Bioaccumulation in Fish: Aqueous and Dietary Exposure) performed on the whole substance indicates BCF values above 10000 (values in the range of 66.5-55 987 depending on the estimation method). Due to the high hydrophobicity of the trimers, the (Q)SAR predictions support high accumulation in fish through uptake via food compared to uptake over the gills.

The trimers are within the applicability domain of the Arnot-Gobas QSAR model and the reliable prediction for the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is a BAF of 177 800, the highest of the trimers. Since 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is predicted to be the most bioaccumulative of the trimers and the OECD TG 305 dietary study indicates BCF values mostly above 10000, 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is considered to fulfil the vB criteria of REACH Annex XIII (BCF > 5000).

Since OAPP contains trimer constituents with B/vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

6.2.1.3 Toxicity

It is not possible with the available information to derive a conclusive decision for the T criterion. No chronic studies on aquatic organisms are available for OAPP or any of its constituents.

6.2.2 Summary and overall conclusions on the PBT and vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH has been used to identify the substance as vPvB. All available relevant information, such as the results of standard tests, monitoring and modelling, information from the application of the analogue approach (read-across) and (Q)SAR results, was considered together in a weight-of-evidence approach.

Oligomerisation and alkylation reaction products of 2-phenylpropene and phenol (OAPP) is a UVCB (substance of Unknown or Variable composition, Complex reaction products and or Biological Materials) consisting of a number of constituents. Some of these constituents are the result of the alkylation of phenols. Others are the result of the oligomerisation of 2-phenylpropene and display relatively similar structures. Within the oligomeric constituents, one of these constituent groups refers to the dimers of 2-phenylpropene, another, to the trimers of 2-phenylpropene.

Persistence
Very limited biodegradation (4% after 28 days) was observed in an OECD TG 310 ready biodegradation study (reliable without restriction) with the whole substance OAPP. Ready biodegradation tests are not capable of discriminating between the relative degradation of each of the constituents and it is hypothesised that strong sorption of some of the extremely lipophilic constituents may reduce the bioavailability to degrading microorganisms. A ready biodegradability test equivalent to OECD TG 301 C (reliable with restrictions) carried out with the dimer of 2-phenylpropene 1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene (EC 228-846-8; CAS 6362-80-7) indicates that the constituent screens as potentially P or vP (0-3% biodegradation after 28 days).

Reliable QSAR predictions for biodegradation (Biowin 2, Biowin 3 and Biowin 6) indicate that all dimers screen as potentially P or vP but more degradation relevant information is generally warranted. As regards the trimers, reliable QSAR predictions for biodegradation using Biowin 2, Biowin 3 and Biowin 6 indicate that all the trimer constituents screen as potentially P or vP.

A reliable without restriction OECD TG 309 test (Aerobic Mineralisation in Surface Water – Simulation Biodegradation Test) was performed on the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4; CAS 3910-35-8) which was chosen as a potential worst-case representative for the dimer fraction. [^{14}C] radiolabelled test material was used and the study conducted over 60 days at two concentrations, 1 and 10 µg/L, at 12 °C. After 60 days, 11.2% and 10.6% mineralisation was reached for the 1 and 10 µg/L concentrations, respectively. One main metabolite was identified in both experiments, 1,3-dimethyl-3-phenyl-2,3-dihydro-1H-indene-1-carboxylic acid. The study indicates that the dimer 1,1,3-trimethyl-3-phenylindan fulfils the P/vP criteria with a half-life in freshwater ≥205 days.

No experimental data is available for the trimers, therefore a read-across approach was

used based on the structural similarity between the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) supported with (Q)SAR results in a weight-of-evidence approach. Based on a read-across approach with the dimer, it can be reasonably assumed that the trimer is at least as persistent as the dimer and thus the degradation half-life in water of the trimer exceeds 60 days. As a consequence, it is concluded that the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC 255-584-1, CAS 41906-71-2) is very persistent in water (degradation half-life >60 days) in accordance with REACH Annex XIII.

Since OAPP contains the dimer 1,1,3-trimethyl-3-phenylindan (EC 223-467-4, CAS 3910-35-8) and the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2) with P/vP properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets both the 'persistence' (P) (degradation half-life in water > 40 days) and 'very persistent' (vP) (degradation half-life in water > 60 days) criteria in accordance with Annex XIII, points 1.1.1 (b) and 1.2.1 (a), of the REACH Regulation.

Bioaccumulation

The dimers and trimers both screen as potentially B and vB with log kow values > 4.5 based on QSAR estimates.

The dimers have shown a potential to reach high levels in fish, both in carp (aqueous OECD TG 305 study performed on CAS 6362-80-7; reliable with restrictions) and in the fathead minnow (dietary OECD TG 305 study performed on the whole substance; reliable without restrictions) where the BCF values ranged from 499—4608 depending on the estimation method (most above 2000). This accumulation is furthermore supported by (Q)SAR predictions.

As regards the trimers, the dietary OECD TG 305 (Bioaccumulation in Fish: Aqueous and Dietary Exposure) performed on the whole substance indicates BCF values above 10000 (values in the range of 66.5-55 987 depending on the estimation method). Due to the high hydrophobicity of the trimers, the (Q)SAR predictions support high accumulation in fish through uptake via food compared to uptake over the gills.

The trimers are within the applicability domain of the Arnot-Gobas QSAR model and the reliable prediction for the trimer 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is a BAF of 177 800, the highest of the trimers. Since 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is predicted to be the most bioaccumulative of the trimers and the OECD TG 305 dietary study indicates BCF values mostly above 10000, 1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan (EC no.: 255-584-1, CAS 41906-71-2) is considered to fulfil the vB criteria of REACH Annex XIII (BCF > 5000).

Since OAPP contains trimer constituents with B/vB properties at a concentration ≥ 0.1 % (w/w), it is concluded that OAPP meets the 'bioaccumulation' criterion (B) and the 'very bioaccumulative' criterion (vB) in accordance with Annex XIII, points 1.1.2 and 1.2.2, of the REACH Regulation.

Conclusion

In conclusion, OAPP is identified as a vPvB substance according to Art. 57(e) of REACH by comparing all relevant and available information listed in Annex XIII of REACH with the criteria set out in the same Annex, in a weight-of-evidence determination. As documented in this report, the trimer (1,3-dimethyl-1-(2-methyl-2-phenyl)propyl-3-phenylindan) (EC 255-584-1, CAS 41906-71-2) present in this UVCB, fulfil the vP criteria as well as the vB criteria.

6.3 Assessment under Article 57(f)

This section is not relevant for the identification of the substance as SVHC in accordance with Article 57 (e) of the REACH Regulation.

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