SUBSTANCE EVALUATION REPORT

Public Name: 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride (Bisphenol A Dianhydride)

EC Number(s): 253-781-7

CAS Number(s): 38103-06-9

Submitting Member State Competent Authority: Germany

Year of evaluation (as given in the CoRAP): 2013

VERSION NUMBER: 1.0 DATE: 19.11.2015

Conclusions of the most recent evaluation step*	Tick relevant box(es)
Concern not clarified; Need to request further information from the Registrant(s) with the draft decision	
Concern clarified; No need of further risk management measures	
Concern clarified; Need for risk management measures; RMO analysis to be performed	
Other: Concern not clarified; No need of further risk management measures because of exposure considerations	x

**Include details in the executive summary.*

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Executive summary

Grounds for concern

Based on the available data in the registration dossier 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride (BPA-DA) fulfills the screening levels of the PBT criteria according to Annex XIII section 3.1 of the REACH regulation. There is a concern that BPA-DA also fulfills the PBT criteria according to annex XIII section 1.2 of the REACH regulation and consequently might be identified as SVHC substance by a more in-depth evaluation.

BPA-DA is not readily biodegradable (0% degradation in 28 d). In addition to that, the production volume is > 100 t/a. Consequently, according to Annex IX of the REACH regulation, simulation tests on degradation in the different media are necessary. Until now requested simulation tests on degradation in water and sediment are missing in the registration dossier. These data, however, are needed to clarify if the persistence criterion is fulfilled.

No measured partition coefficient n-octanol/water (log Pow) for BPA-DA is included in the registration dossier. A read-across to the primary hydrolysis product (4,4-Bisphenol A Tetra-Acid, BPA-TA, CAS 38103-05-8) was made by the registrant. The respective log Pow of BPA-TA ranges from 5.02 to < -2.2 depending on pH. The estimated log Pow of 6.851 for BPA-DA is higher and indepent from pH. Consequently, the read across to the BPA-TA seems not to be reasonable. A log Pow > 4.5 indicates a high potential for bioaccumulation and according to Annex IX a bioaccumulation study is necessary.

Based on the information available for the P and B endpoints in the registration dossier, an assessment of the PBT-properties is difficult, because standard data requirements of Annex IX are missing. The substance is registered for a high aggregated tonnage band of > 1000 t/a. Consequently, a PBT assessment seems to be appropriate in this case.

Procedure

Environment

The initial concern is based on a screening concerning the PBT properties. These properties were identified by a QSAR screening and prioritization exercise of some MSs and ECHA. Based on these findings the substance evaluation was justified (Justification for the selection of a candidate CoRAP substance). Substance evaluation started in March 2013 based on an aggregated data set submitted by the registrant(s) for the substance registration in 2010 under REACH. Referred to the screening 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride (BPA-DA) fulfils the screening levels of the PBT criteria. Accordingly, the evaluation targeted the persistency, the bioaccumulation potential and toxicity. As the T criterion is based on an aquatic NOEC for pelagic organisms, the terrestrial compartment and terrestrial toxicity was not subject of this substance evaluation. The first substance evaluation draft decision of 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride (BPA-DA) was sent to registrants in May 2014.

Comments from the registrant were received in June 2014 and an update of the registration dossier in February 2015 plausibly demonstrated that the substance is only imported as a reacted monomer in polymers and that the percentage of the residual monomer in polymers is <0.1% w/w. Thus, the percentage of the monomer is below the threshold to identify the polymer as PBT substance. A clarification of the PBT-status of the monomer by means of a substance evaluation would not lead

to further regulatory measures. For the same reason it was concluded that exposure to the environment is of no relevance. Consequently, DE as evaluating MS did not consider the requesting of further information as necessary. On that basis, the decision-making process was terminated and the substance evaluation concluded.

Therefore, the concern for potential PBT properties remains unverified since no additional information was requested to clarify the concern due to the termination of the substance evaluation decision making process.

Conclusions

The P-criterion cannot finally be assessed for BPA-DA and its hydrolysis product BPA-TA because half life values for the environmental compartments are missing.

The screening criterion for B is met for BPA-DA, because the estimated Log Kow > 4.5. Consequently, the substance is potentially B but experimental BCF data are missing. For the hydrolysis product BPA-TA no conclusion for B is possible because necessary screening data and measured bioaccumulation data are missing.

There are no toxicity data given for BPA-DA. Based on the information provided by the registrant for the hydrolysis product BPA-TA it cannot be excluded with certainty that the T-criterion is fulfilled as chronic data are missing.

In line with the justification document, the endpoints persistence as well as bioaccumulation of BPA-DA were evaluated. Based on the available information both criteria could not be clarified. According an update of the registration dossier in February 2015 the substance is only imported as a reacted monomer and the percentage of the residual monomer is <0.1% w/w. Thus, the percentage of the monomer is below the threshold to identify the polymer as PBT substance. A potential verification of the PBT-status of the monomer by means of a substance evaluation would not lead to further regulatory measures. For the same reason it is concluded that exposure to the environment is of no relevance. Therefore, the substance evaluation has been concluded at this point.

CONTENTS

TABLES

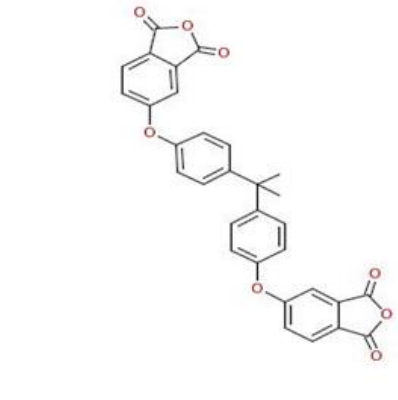
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 1: Substance identity

Public Name:	4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride
EC number:	253-781-7
EC name:	4,4'-((Isopropylidene)bis(p-phenyleneoxy))diphthalic dianhydride
CAS number (in the EC inventory):	38103-06-9
CAS number:	38103-06-9
CAS name:	
IUPAC name:	5,5'-(Propane-2,2-diylbis(4,1-phenyleneoxy))bis(2-benzofuran-1,3-dione)
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	C31H20O8
Molecular weight or molecular weight range:	520.4857
Synonyms:	1,3-Isobenzofurandione, 5,5'-((1-methylethylidene)bis(4,1-phenyleneoxy))bis-

Structural formula:



1.2 Composition of the substance

Name: 4,4'-((Isopropylidene)bis(p-phenyleneoxy))diphthalic dianhydride (BPA-DA)

Description: mono constituent substance, organic

Degree of purity: confidential

Table 2: Constituents

Constituents	Typical concentration	Concentration range	Remarks
4,4'-((Isopropylidene)bis(p-phenyleneoxy))diphthalic dianhydride, EC 253-781-7	confidential	confidential	The isomers of CAS No. 38103-06-9 (EC No. 253-781-7) should be considered as impurities and not as part of the substance.

Table 3: Impurities

Impurities	Typical concentration	Concentration range	Remarks
-			

Table 4: Additives

Additives	Typical concentration	Concentration range	Remarks
-			

1.3 Physico-chemical properties

Table 5: Overview of physicochemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	cream colored solid	*Discussion and the value used for Chemical Safety Assessment (CSA) reported in the endpoint summary*
Melting/freezing point	185 – 190 °C	Capillary tube in a metal block, according to OECD 102
Boiling point	>314 °C at 1013 hPa	Capillary method, according to OECD 103
Density	1.31 g/cm3 at 21 °C	Pycnometer method, OECD 109
Vapour pressure	5E-18 Pa at 25 °C	Calculated based on its boiling point by computer software from Advanced Chemistry Development Inc.
Surface tension	*idem*	In accordance with Column 2 of REACH, Annex VII, Section 7.6, the study does not need to be conducted when, based on the chemical structure, surface activity is not expected.
Water solubility	*idem*	In accordance with Column 2 of REACH, Annex VII, section 7.7, the water solubility study does not need to be conducted if the substance is hydrolytically unstable at pH 4, 7 and 9. Data show that BPA-DA is hydrolytically unstable, with a half-life less than 12 hours.
Partition coefficient n-octanol/water (log value)	Pow=5.02, log Pow= 0.7 at pH 5 and 21 °C; Pow< 0.00698, log Pow= -2.22 at pH 7 and 21 °C Pow=<0.00732, log Pow <-2.2 at pH 9 and 21 °C	The test substance is not the same as the substance being registered: BPA-DA was determined to be hydrolytically unstable at pH 2, pH 5-6, and pH 9 (Vizon SciTec Inc., 2005), therefore the partition coefficient test was conducted with the hydrolysis product, 4,4-Bisphenol Tetra-Acid (BPA-TA; CAS 38103-05-8).
Flash point	*idem*	*idem*
Flammability	*idem*	*idem*
Explosive properties	*idem*	*idem*
Self ignition temperature	*idem*	*idem*
Oxidising properties	*idem*	*idem*
Granulometry	9% of the particles > 150 µm; no particles < 38 µm	*Sieve analysis*

Stability in organic solvents and identity of relevant degradation products	*idem*	In accordance with Column 1 of Annex IX, section 7.15, the study is not required as the stability of the substance in organic solvents is not considered critical.
Dissociation constant	*idem*	In accordance with Column 2 of Annex IX, section 7.16, the study does not need to be conducted when the test substance is hydrolytically unstable with a half-life that is less than 12 hours. Therefore, no testing for dissociation constant is required.
Viscosity	*idem*	In accordance with the REACH information requirements R.7A, R.7.1.18.4, viscosity testing is not relevant for substances that are not a liquid at room temperature. Therefore, no testing for viscosity is required.
Auto flammability	*idem*	*idem*
Reactivity towards container material	*idem*	*idem*
Thermal stability	*idem*	*idem*

2 MANUFACTURE AND USES

2.1 Quantities

Table 6: Aggregated tonnage (per year)

1 – 10 t	10 – 100 t	100 – 1000 t	1000- 10,000 t X	10,000-50,000 t
50,000 – 100,000 t	100,000 – 500,000 t	500,000 – 1000,000 t	> 1000,000 t	Confidential

2.1.1 Manufacturing processes

2.2 Identified uses

BPA-DA is a "monomer" that is present only as a reacted component of an imported polymer and therefore the substance itself has no use pattern within the EU.

2.2.1 Uses by workers in industrial settings

confidential

3 CLASSIFICATION AND LABELLING

3.1 Harmonised Classification in Annex VI of the CLP Regulation

Not applicable

3.2 Self classification

Classification		Labelling		Specific Concentration limits, M- Factors
Hazard Class and Category Code(s)	Hazard Statement Code(s)	Hazard Statement Code(s)	Supplementary Hazard Statement Code(s)	
Skin Irrit. 2	H315	H315		
Eye Irrit. 2	H319	H319		
Resp. Sens. 1	H334	H334		
STOT SE 3	H335	H335		

Signal Words: Danger **Pictograms**: GHS07, GHS08

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Abiotic degradation

4.1.1.1 Hydrolysis

Due to its structure, BPA-DA is expected to readily hydrolyze in water. This assumption is confirmed by the experimental data given in the registration dossier.

BPA-DA was determined to be hydrolytically unstable at pH 2, 5-6 and 9 at 23 degrees C in an OECD 111 test (2005: Unpublished study record, confidential). The estimated BPA-DA half-lives were obtained at high acetonitrile cosolvent concentration. First order half lives of BPA-DA in acetonitrile/aqueous solution (60/40, v/v) are 1.5h, 2.0h, 2.5h at pH 4, 7 and 9, respectively, at 23 degrees C.

A preliminary test according to OECD 111 was conducted on the primary hydrolysis product 4,4'-Bisphenol A Tetra Acid (BPA-TA). The half-life as extrapolated from that test at 50 degrees C is > 1 yr, at pH 4, 7 and 9 at ambient conditions (2009: Unpublished study record, confidential).

4.1.1.2 Phototransformation/photolysis

4.1.1.2.1 Phototransformation in air

The registration dossier contains a calculated half-life in air of 8.062 h under 12 hour daylight conditions for BPA-DA, based on reaction with hydroxyl radicals. The documentation of this QSAR result does not comply with REACH Annex XI and thus its reliability is limited. This result is not considered further as it is not relevant for this dossier.

4.1.2 Biodegradation

4.1.2.1.1 Screening tests

The registration dossier contains one study on ready biodegradation conducted according to OECD guideline 301D. No biodegradation of BPA-DA was observed: -1.6 % degradation of BPA-DA occurred over a 28 day test period at 19.8-20.9 degrees C (Aerobic, non-renewal, degradation products were not measured).

Since BPA-DA hydrolyzes to BPA-TA readily and the observed half-life is about 2 hours, it is possible that the hydrolysis product BPA-TA was formed in the 28 day Ready Biodegradation test and that BPA-TA is also not readily biodegradable.

4.1.2.1.2 Summary and discussion of biodegradation in water and sediment

In pure water, BPA-DA is not stable and hydrolyzes relatively fast (within hours) to form 4,4'-Bisphenol A Tetra Acid (BPA-TA; CAS 38103-05-8). However, in a water-sediment system, this hydrolysis reaction may be delayed significantly by sorption to particles.

BPA-TA is not sensitive to hydrolysis. No degradation was observed in a test on Ready biodegradability, indicating that BPA-DA and BPA-TA is not ready biodegradable.

Consequently, both BPA-DA and BPA-TA are regarded as potentially persistent.

4.1.3 Summary and discussion on degradation

In pure water, BPA-DA is not stable and hydrolyzes relatively fast (within hours) to form 4,4'-Bisphenol A Tetra Acid (BPA-TA). However, in a water-sediment system, this hydrolysis reaction may be delayed significantly by sorption to particles.

BPA-TA is not sensitive to hydrolysis. No degradation was observed in a test on Ready biodegradability, indicating that BPA-DA and BPA-TA is not ready biodegradable.

In conclusion, both BPA-DA and its hydrolysis product BPA-TA are considered to fulfil the screening criterion for persistency. However, no simulation tests on biodegradation in environmental compartments are available. Further testing on biodegradability would be required to conclude whether BPA-DA and BPA-TA are persistent or very persistent according to REACH Annex XIII.

4.2 Bioaccumulation

4.2.1 Aquatic bioaccumulation

Screening Information

No experimental log Kow value is available. The estimated log Kow (8.87, KOWWIN v.1.68, not documentation according Annex 11) of BPA-DA indicates a high potential for bioaccumulation.

The hydrolysis product BPA-TA is a tetraprotic acid. Thus, the substance dissociates under environmental relevant pH conditions (pH 4-9). For dissociated substances Log D instead of Log Kow should be used as screening information for the bioaccumulation potential. As no Log D values are available for BPA-TA, the potential for bioaccumulation cannot be assessed.

Measured Data

No measured bioaccumulation data are available.

4.2.2 Terrestrial bioaccumulation

No experimental data are available.

4.2.3 Summary and discussion of bioaccumulation

The estimated Log Kow of BPA-DA exceeds the screening criteria of 4.5 and therefore indicates a high potential for bioaccumulation. No measured bioaccumulation data are available. A final assessment of the bioaccumulation potential of BPA-DA is not possible.

The hydrolysis product BPA-TA dissociates under environmental relevant pH conditions. Therefore, Log D instead of Log Kow is needed as screening information for the bioaccumulation potential but is not available. As in addition no measured bioaccumulation data are available, a final assessment of the bioaccumulation potential of the hydrolysis product is not possible.

5 ENVIRONMENTAL HAZARD ASSESSMENT

The test substance BPA-DA hydrolyses in water within hours. Therefore, the registrant only provides toxicity data on the hydrolysis product BPA-TA.

5.1 Aquatic compartment (including sediment)

5.1.1 Toxicity data

Data for the acute toxicity of BPA-TA are available for all three trophic levels (fish, Daphnia, algae).

5.1.1.1 Fish

5.1.1.1.1 Short-term toxicity to fish

Acute Toxicity of the hydrolysis product BPA-TA was determined according to the OECD 203 guideline with Rainbow trout (*Oncorhynchus mykiss*). The observed LC 50 is > 116 mg/l based on the measured concentration.

5.1.1.1.2 Long-term toxicity to fish

There are no data available.

5.1.1.2 Aquatic invertebrates

5.1.1.2.1 Short-term toxicity to aquatic invertebrates

An acute toxicity test was conducted with the hydrolysis product BPA-TA according to OECD 202 with daphnia magna. The exposure time was extended to 96 h instead of 48 h and thus the test procedure of OECD 202 was modified. The observed EC 50 is > 1248 mg/l based on the measured concentration.

5.1.1.2.2 Long-term toxicity to aquatic invertebrates

There are no data available.

5.1.1.3 Algae and aquatic plants

The algae *Pseudokirchnerella subcapitata* were tested according to the OECD 201 guideline. The test procedure was modified prolonging the exposure time to 96 h. The EC50 of the hydrolysis product BPA-TA based on growth inhibition is 1713 mg/l and the NOEC < 877mg/l.

5.1.1.4 Sediment organisms

There are no data available.

5.1.2 Calculation of Predicted No Effect Concentration (PNEC)

5.1.2.1 PNEC water

Not evaluated.

5.1.2.2 PNEC sediment

Not evaluated.

5.2 Terrestrial compartment

5.2.1 Toxicity test results

5.2.1.1 Toxicity to soil macro organisms

There are no data available.

5.2.1.2 Toxicity to terrestrial plants

5.2.1.3 There are no data available. Toxicity to soil micro-organisms

There are no data available.

5.2.1.4 Toxicity to other terrestrial organisms

There are no data available.

5.2.2 Calculation of Predicted No Effect Concentration (PNEC soil)

Not evaluated.

5.3 Atmospheric compartment

Not evaluated.

5.4 Endocrine disrupting properties

Not evaluated.

5.5 Microbiological activity in sewage treatment systems

Not evaluated.

5.5.1 Toxicity to aquatic micro-organisms

There are no data available.

5.5.2 There are no data available. PNEC for sewage treatment plant

Not evaluated.

5.6 Non compartment specific effects relevant for the food chain (secondary poisoning)

Not evaluated.

5.6.1 Toxicity to birds

Not evaluated.

5.6.2 Toxicity to mammals

Not evaluated.

5.6.3 Calculation of PNECoral (secondary poisoning)

Not evaluated.

5.7 Conclusion on the environmental hazard assessment and on classification and labelling

Not evaluated.

6 PBT AND VPVB ASSESSMENT

6.1 Assessment of PBT/vPvB properties – Comparison with the criteria of Annex XIII

6.1.1 Persistence assessment

In pure water, BPA-DA is not stable and hydrolyzes relatively fast (within hours) to form 4,4'-Bisphenol A Tetra Acid (BPA-TA). BPA-TA is not sensitive to hydrolysis.

No degradation was observed in a test on Ready biodegradability, indicating that BPA-DA and the hydrolysis product BPA-TA are not ready biodegradable.

In conclusion, BPA-DA and the degradation product BPA-TA are considered to fulfil the screening criterion for persistency. However, no simulation tests on biodegradation in environmental compartments are available. Further testing on biodegradability would be required to conclude whether BPA-DA or its hydrolysis product BPA-TA are persistent or very persistent according to REACH Annex XIII.

6.1.2 Bioaccumulation assessment

The estimated Log Kow of BPA-DA exceeds the screening criterion of 4.5 and therefore is considered as potentially B. No measured bioaccumulation data are available. Consequently, comparison of experimental BCF values with the criteria of Annex XIII is not possible.

The hydrolysis product BPA-TA dissociates under environmental relevant pH conditions. Therefore, Log D instead of Log Kow is needed as screening information for the bioaccumulation potential but is not available. As in addition no measured bioaccumulation data are available, the assessment of the bioaccumulation potential of the hydrolysis product is not possible.

6.1.3 Toxicity assessment

There are no toxicity data given for BPA-DA. Consequently, a toxicity assessment is not possible. Therefore, the following the toxicity assessment is conducted with hydrolysis product BPA-TA.

For the hydrolysis product BPA-TA only data from acute tests are available, with the exception of the algae study which can be regarded as a chronic test. Based on the acute eco-toxicity data the screening criterion for T (EC/LC < 0.1. mg/l) is not met. According to Section 1.1.3 of Annex XIII to REACH Regulation, a substance is considered to fulfil the toxicity criterion (T) when the long-term no-observed effect concentration (NOEC) / EC10 for marine or freshwater organisms is less than 0.01 mg/l. A conclusion concerning the toxicity cannot be drawn on the basis of acute data. With a given NOEC less than 877mg/l for algal growth an actual NOEC-value is not given and a clear conclusion cannot be drawn.
Based on the information provided by the registrant, it cannot be excluded with certainty that the BPA-TA fulfils the T-criterion as chronic data are missing.

6.1.4 Summary and overall conclusions on PBT and vPvB Properties

The P-criterion cannot be assessed for BPA-DA and the hydrolysis product BPA-TA because both substances are not readily biodegradable but half life values for the environmental compartments are missing.

The screening criterion for B is met for BPA-DA, because of the estimated Log Kow > 4.5. Consequently, the substance is potentially B. As experimental BCF values are missing no final conclusion is possible for BPA-DA. For the hydrolysis product BPA-TA no conclusion for B is possible because necessary screening data (LogD values) and measured bioaccumulation data are missing.

There are no toxicity data given for BPA-DA. Consequently, an assessment of the toxicity is not possible. Based on the information provided by the registrant for the hydrolysis product BPA-TA it cannot be excluded with certainty that the T-criterion is fulfilled as chronic data are missing.

7 EXPOSURE ASSESSMENT

BPA-DA has been registered for a tonnage band >1.000 t/a. The initial concern for performing a substance evaluation of BPA-DA was the PBT potential in the environment. BPA-DA is a "monomer" that is present only as a reacted component of an imported polymer and therefore the substance itself has no use pattern within the EU. It is registered in accordance with Article 6 (3) of REACH. Taking into account registrants´ information, it is concluded that the release of BPA-DA into the environment is negligible. Hence, the data analysed with respect to exposure issues during the substance evaluation of BPA-DA did not support our conclusion that BPA-DA is an environmentally relevant contaminant in aqueous media.

8 REFERENCES

Title	Author	Publication/source details	Date
Molecular size cutoff criteria for screening bioaccumulation potential: Fact or fiction?	Arnot, J.A., Arnot, M.I., Mackay, D., Couillard, Y., MacDonald, D., Bonnell, M., Doyle	Integrated Environmental Assessment and Management 6, 210-224	2010
Identifying New Persistent and Bioaccumulative Organics Among Chemicals in Commerce	Howard, P.H., Muir, D.C.G.	Environmental Science & Technology 44, 2277-2285	2010
Are there other persistent organic pollutants? A challenge for environmental chemists.	Muir, D.C.G., Howard, P.H.	Environmental Science & Technology 40, 7157-7166	2006
The Physical Properties Database	Beauman, J. A.; Howard, P. H.	Syracuse Research Corporation	2001 (Accessed on July 2013)