Justification Document for the Selection of a CoRAP Substance

Group Name: Diisoquinoline tetrones

EC	CAS	Substance public name
201-344-6	81-33-4	Perylene-3,4:9,10-tetracarboxydiimide
226-866-1	5521-31-3	2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone

Authority: BE CA

Date: 19/03/2019

Cover Note

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

1 IDENTITY OF THE SUBSTANCES WITHIN THE GROUP

1.1 Other identifiers of the substances within the group

EC name (public)	IUPAC name (public)	Index number in Annex VI of the CLP Regulation	Molecular formula	Molecular weight or molecular weight range	Synonyms
Perylene-3,4:9,10-tetracarboxydiimide	7,18-diazaheptacyclo[14.6.2.2^{2,5}.0^{3,12}.0^{4,9}.0^{13,23}.0^{20,24}]hexacosa-1(23),2,4,9,11,13,15,20(24),21,25-decaene-6,8,17,19-tetrone	NA	$C_{24}H_{10}N_2O_4$	390.3	3,4,9,10-perylenetetracarboxylic 3,4:9,10-diimide 3,4,9,10-Perylenetetracarboxylic 3,4:9,10-diimide (6CI, 7CI, 8CI) 3,4,9,10-Perylenetetracarboxylic acid diimide 3,4,9,10-Perylenetetracarboxylic diimide 3,4,9,10-Perylentetracarbonsäurediimid 3,4,9,10-Perylentetracarboxyldiimid Anthra[2,1,9-def:6,5,10-

					d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone (9CI) Anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetron e (9CI) anthra[2,1,9-def:6,5,10-d¿e¿f¿]diisoquinoline-1,3,8,10(2H,9H)-tetrone C.I. 71129 C.I. Pigment Violet 29 Perylimid Perylimid L (BASF) PV-Fast Bordeaux B
2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone	7,18-dimethyl-7,18-diazaheptacyclo[14.6.2.$2^{2,5}$.$0^{3,12}$.$0^{4,9}$.$0^{13,23}$.$0^{20,24}$]hexacosa-1(22),2,4,9,11,13(23),14,16(24),20,25-decaene-6,8,17,19-tetrone	NA	$C_{26}H_{14}N_2O_4$	418.4	3,4,9,10-Perylenetetracarboxylic 3,4:9,10-bis(N-methylimide) 3,4,9,10-Perylenetetracarboxylic 3,4:9,10-diimide, N,N'-dimethyl- (7CI, 8CI)

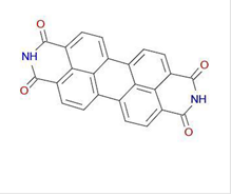
					Anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone, 2,9-dimethyl-(9CI) Anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone, 2,9-dimethyl-(9CI) C.I. 71130 C.I. Pigment Red 179 C.I. Vat Red 23 Hostaperm-Rot P2GL Indanthren Rot FGL N,N'-Dimethyl-3,4,9,10-perylenetetracarboxylic diimide N,N'-Dimethylperylene-3,4,9,10-tetracarboxylic 3,4:9,10-diimide N,N'-Dimethylperylene-3,4,9,10-tetracarbox

					ylic acid diimide N,N'-Dimethylperylene-3,4:9,10-bis(dicarboximide) N-Methyl-3,4,9,10-perylenetetracarboxyldiimide Paliogen Maroon L 3820 Paliogen Maroon L 3920 Paliogen Maroon L 4020 Paliogen Rot 4120 Pulver (BASF) Perylene 3,4,9,10-tetracarboxylic acid bis(methylimide)

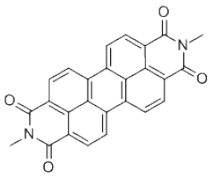
Type of substances ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

Structural formulas:

EC 201-344-6



EC 226-866-1



1.2 Similar substances/grouping possibilities

NA

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

other processes	RMOA	REACH process			Authorisation		Restriction	h C&L	process under other EU legislation		previous legislation		Stockholm convention	other processes EU legislation
EC entries		CCH	TPE	SEV	candidate list	Annex XIV	Annex XVII	Annex VI (CLP)	PPP	BPR	NONS	RAR	POPs	
201-344-6	/	/	/	/	/	/	/	/	/	/	/	/	/	Manual screening
226-866-1	/	/		/	/	/	/	/	/	/	/	/	/	Manual screening

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

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3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

NA

3.1.2 Self classification

- In the registration:

Both substances are not classified in the registration.

- The following hazard classes are in addition notified among the aggregated self classifications in the C&L Inventory:

EC Nr	C&L Inventory	
	Hazard class category code	**Hazard statement code**
201-344-6	Not classified	/
226-866-1	Skin Irrit. 2 Eye irrit. 2 STOT SE 3	H315: Causes skin irritation H319: Causes serious eye irritation H335: May cause respiratory irritation

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

NA

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[1]

4.1 Tonnage and registration status

Table: Tonnage and registration status

Substance EC 201-344-6 and 226-866-1

From ECHA dissemination site *		
☒ Full registration(s) (Art. 10)	☐ Intermediate registration(s) (Art. 17 and/or 18)	
Tonnage band (as per dissemination site)		
☐ 1 – 10 tpa	☐ 10 – 100 tpa	☒ 100 – 1000 tpa
☐ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ 10,000,000 – 100,000,000 tpa	☐ > 100,000,000 tpa
☐ <1 . . . . . >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa)		☐ Confidential

***the total tonnage band has been calculated by excluding the intermediate uses, for details see the Manual for Dissemination and Confidentiality under REACH Regulation (section 2.6.11): https://echa.europa.eu/documents/10162/22308542/manual_dissemination_en.pdf/7e0b87c2-2681-4380-8389-cd655569d9f0

4.2 Overview of uses

Table: Uses (in three parts)

Part 1:

Substance: 201-344-6						
☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☒ Consumer use	☒ Article service life	☐ Closed system
Substance: 226-866-1						
☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☒ Consumer use	☒ Article service life	☐ Closed system

[1] Dissemination website consulted on 20 July 2018

Part 2:

Substance1: EC 201-344-6

	Use(s)	Technical function
Uses as intermediate	/	/
Formulation	Use as laboratory reagent Industrial formulation of non-solid preparations containing pigment (including inks and paints) Formulation into solid matrix Coatings and inks – manufacture of organic solvent borne, water bonrne and solvent-free products Industrial formulation of solid preparations containing pigment (including plastics) Coatings and inks – manufacture of powder products	
Uses at industrial sites	Coatings and inks application-industrial Industrial removal of matrix (e.g. abrasion) Industrial use of pigment preparations resulting in inclusion into a matrix (including ink and paint) Use in laboratory Industrial use of pigment preparations resulting in inclusion into a matrix (including plastic) Use at industrial site leading to inclusion into/onto article	
Uses by professional workers	Widespread use leading to inclusion into/onto article (indoor and outdoor) Professional removal of matrix, outdoor and indoor (e.g. abrasion) Coatings and inks application – professional	
Consumer Uses	Consumer outdoor and indoor use of pigmented articles with low release Widespread use leading to inclusion into/onto article (indoor and outdoor) Consumer removal of matrix, outdoor and indoor (e.g. abrasion) Coatings – consumer application of coatings	
Article service life	Worker and consumer use of plastic articles Removal of matrix (e.g. abrasion, indoor and outdoor): Worker and consumer use of verhicles, metal articles, wood articles and painted articles Outdoor and indoor use of coloured articles: Metal, paper, wood, plastic and painted articles	

Substance2: EC: 226-866-1

	Use(s)	Technical function
Uses as intermediate	/	/
Formulation	Coatings and inks – manufacture of powder products Formulation into solid matrix Industrial formulation of solid preparations containing pigment (including plastics) Use in laboratory Coatings and inks – manufacture of organic solvent borne, water borne and solvent-free products Industrial formulation of non-solid preparations containing pigment (including inks and paints)	
Uses at industrial sites	Industrial use of pigment preparations resulting in inclusion into a matrix (including plastic, ink and paint) Coatings and inks application Industrial removal of matix (e.g. abrasion) Use in laboratory	
Uses by professional workers	Widespread dispersive outdoor and indoor use resulting in inclusion into a matrix Professional removal of matrix, indoor and outdoor (e.g. abrasion) Coatings and inks application	
Consumer Uses	Widespread dispersive outdoor use resulting in inclusion into a matrix: Coatings and paints, thinners, paint removes, pigment and pigment additives Indoor and outdoor use of pigmented articles with low release Widespread dispersive indoor use resulting in inclusion into a matrix: Coatings and paints, thinners, paint removes, ink and toners, pigment and pigment additives Outdoor use of pigmented articles with low release Consumer application of coatings: Coatings and paints, thinners, paint removes, fillers, putties, plasters, modelling clay, finger paints Removal of matrix, indoor and outdoor (e.g. abrasion)	
Article service life	Consumer use of plastic articles Consumer outdoor and indoor use of coloured articles: metal, paper, wood, plastic and painted articles Workers and consumers removal of matrix (e.g. abrasion), outdoor and indoor: Vehicles, metal articles, wood articles and painted articles	

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE OR GROUP

5.1. Legal basis for the proposal

☒ Article 44(2) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

5.2. Selection criteria met (why the substance or group qualifies for being in CoRAP)

☐ Fulfils criteria as CMR/ Suspected CMR

☐ Fulfils criteria as Sensitiser/ Suspected sensitiser

☐ Fulfils criteria as potential endocrine disrupter

☒ Fulfils criteria as PBT/vPvB / Suspected PBT/vPvB

☐ Fulfils criteria high (aggregated) tonnage (*tpa > 1000*)

☒ Fulfils exposure criteria

☐ Fulfils MS's (national) priorities

5.3 Initial grounds for concern to be clarified under Substance Evaluation

Hazard based concerns		
CMR ☐ C ☐ M ☐ R	Suspected CMR[1] ☐ C ☐ M ☐ R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[2]	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[1]	☐ Other (please specify):
Exposure/risk based concerns		
☐ Wide dispersive use	☐ Consumer use	☐ Exposure of sensitive populations
☐ Exposure of environment	☐ Exposure of workers	☐ Cumulative exposure
☐ High RCR	☐ High (aggregated) tonnage	☐ Other (please specify below)
The registration dossiers of Perylene-3,4:9,10-tetracarboxydiimide and 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone are built upon the grouping strategy (using category of solid pigments derived from central perylenetetracarboxyl moiety which differ from one another by the various substituents), and the members of this group are then further used for the read-across purposes. From the perspective of the physico-chemical characteristics the differences between the group members are more or less negligible. It is also deemed unlikely that the two substances show different ecotoxicological effects. Therefore a read-across approach between the 2 substances seems to be appropriate for environmental endpoints.		

The registrants state in their dossier that the substances are neither soluble in water nor soluble in organic solvents, therefore a very low bioavailability is expected. BE CA considers however that the reliability of the water solubility and partition coefficient data for Perylene-3,4:9,10-tetracarboxydiimide as questionable. The registration dossier for this substance indicates that water solubility of 0.01 mg/L at 20° C, while EpiSuite presents two estimation methods for water solubility : WSKOW v.1.42 ➔ 6.3 mg/L; Wat Sol v1.01 ➔ 0.64 mg/L. In both estimation methods the various fragments are recognized and the molecular weight is in the applicability domain. Therefore these estimation methods should be accepted in a weight-of-evidence approach. In addition the registration dossier of 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone contains two divergent values of water solubilty - 5.5 µg/L based on ETAD method and 20 µg/L used for calculation of log K_{ow}. Estimated values from EpiSuite for water solubility of 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone are as follows: WSKOW v.1.41 - 6.3 mg/L; WATERNT v1.01 - 0.006 mg/L.

Because the estimated values substantially diverge from the value given in the registration dossier and because water solubility is a crucial element, it seems appropriate not to use the value presented by REG as an argument to deny the B-concern. Regarding log Kow value, the registrants indicated that the log K_{ow} could only be calculated based on the measured solubility and the log Kow value of 0.85 at 25° C is used for further assessments. EPI Suite however estimates significantly higher value of log Kow = 1.92. Therefore in the view of BE CA, a reliable conclusion on the bioavailability of this substance is not possible based on the currently available data.

PBT assessment:

For both substances in the group, definitive information on persistence (simulation studies / half-lives) is not available. Screening information does not indicate (bio)degradation. In view of the structure of the substances, it is reasonable to expect that the P and the vP criterion are met for these substances and QSAR estimations support this concern.

BE CA observes that the assessment from the Registrants does not consider the possibility that in field conditions (slow) degradation of the parent compounds takes place. The core diisoquinoline structures are probably quite stable, but it should be considered whether the imide-functionalities can react either abiotically or by biodegradation. If these compounds "lose" their functional groups, the log K_{ow}-values of the degradation products will become much higher and the screening criterion for B will certainly be met. Additionally, it should also be considered that the perylene core of these diisoquinolines is a PAH which shows a structural similarity with PAHs as there are :

1. benz[a]anthracene (EC 200-280-6)(identified as carcinogenic, PBT & vPvB),

2. chrysene (EC 205-923-4)(identified as carcinogenic, PBT & vPvB),

3. Benzo[a]pyrene (EC 200-028-5)(identified as carcinogenic, mutagenic, toxic for reproduction, PBT & vPvB)

Experimental studies on bioaccumulation are not available, nor for aquatic organisms, nor for terrestrial organisms and mammals. In the absence of relevant studies, current evaluation can only refer to screening criteria. In this framework the log K_{ow} and log K_{oa}-values are important metrics. For perylene-3,4:9,10-tetracarboxydiimide, the following values are estimated by EpiSuite : log K_{ow} = 1.92, log K_{oa} = 20.7. Based on these estimated values, the B screening criterion for aquatic organisms is not fulfilled. On the contrary, the estimated log K_{oa}-value is extremely high what indicates a high potential for bioaccumulation in air-breathers (ECHA Guidance Chapter R.11: PBT/vPvB assessment). Based on this observation

[2] CMR/Sensitiser: known carcinogenic and/or mutagenic and/or reprotoxic properties/known sensitising properties (according to CLP harmonized or registrant self-classification or CLP Inventory)
Suspected CMR/Suspected sensitiser: suspected carcinogenic and/or mutagenic and/or reprotoxic properties/suspected sensitising properties (not classified according to CLP harmonized or registrant self-classification)
Suspected PBT: Potentially Persistent, Bioaccumulative and Toxic

the substance may accumulate in terrestrial organisms and in mammals. The same conclusion applies also to 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone (log K_{oa} = 20.4 from EpiSuite estimation).

In support of the above mentioned, the registration dossier of 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone contains two divergent values of log K_{ow}: 2.68 and -0.03. Log K_{ow} value of 4.18 was calculated using EpiSiute and another Log K_{ow} value of 1.87 ± 0.97 was calculated using ACD/Percepta 14.2.0 (Build 2977), but the latter result has been calculated with a high degree of uncertainty.

Another parameter that can provide information on the bioaccumulation potential is the average maximum diameter (Dmax,ave); Compounds with a Dmax,aver, greater than 1.7 nm are unlikely to meet the BCF-criterion because they are too bulky. Based on a simple calculation method, the maximum diameters of Perylene-3,4:9,10-tetracarboxydiimide and 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone are 1.4 and 1.6 nm, respectively. Therefore these molecular dimensions do not suggest the substances to be non-bioaccumulative.

Regarding T assessment, only acute ecotoxicity studies are available. In these studies no indications are found that the substances meet the eco-T criterion.

The substances are not self-classified for carcinogenicity, germ cell mutagenicity, toxicity for reproduction or STOT RE, hence based on the current data the T criterion for human health is not fulfilled.

Taking into account the wide dispersive use, high tonnage and the environmental exposure of Perylene-3,4:9,10-tetracarboxydiimide and 2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H) –tetrone, a potential risk the environment cannot be excluded. Therefore, the concern regarding persistence and bioaccumulation should be addressed under substance evaluation procedure.

5.4 Indication of information that may need to be requested to clarifyfy the concern

☒ Information on toxicological properties	☒ Information on physico-chemical properties
☒ Information on fate and behaviour	☐ Information on exposure
☐ Information on ecotoxicological properties	☐ Information on uses
☐ Information on ED potential	☐ Other (provide further details below)
The biodegradation potential will first be further analysed. If the P-character is confirmed, experimental testing on bioaccumulation could be envisaged (potentially via toxicikinetics study).	

5.5 Potential follow-up and link to risk management

☐ Harmonised C&L	☐ Restriction	☒ Authorisation	☐ Other (provide further details)
In case that the concern for persistency and bioaccumulation are confirmed, the identification of both substances as SVHC according to article 57 (e) of REACH would be a potential follow-up measure in order to improve the RMMs for these substances.			