Justification Document for the Selection of a CoRAP Substance

Substance Name (public name):	Esterification products of 1,3-dioxo-2-benzofuran-5-carboxylic acid with nonan-1-ol
EC Number:	941-303-6
CAS Number: -	
Authority:	France
Date:	21/03/ 2017

Cover Note

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

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1 IDENTITY OF THE SUBSTANCE

1.1 Other identifiers of the substance

Table: Other Substance identifiers

EC name (public):	Esterification products of 1,3-dioxo-2-benzofuran-5-carboxylic acid with nonan-1-ol
IUPAC name (public):	-
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	not applicable, UVCB substance
Molecular weight or molecular weight range:	-
Synonyms:	DIPLAST® TM 9

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

Structural formula:

Other relevant information about substance composition

Table: Constituent

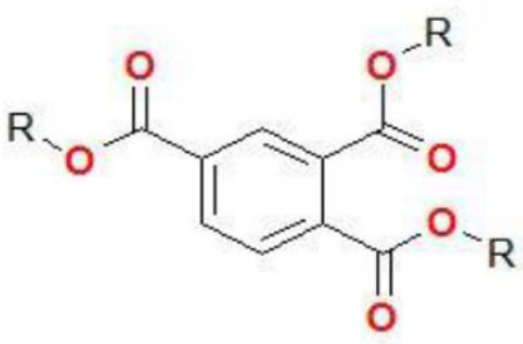
EC number:	941-303-6
EC name (public):	-
CAS number:	-
CAS name (public):	-
IUPAC name (public):	-
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	not applicable, UVCB substance
Molecular weight or molecular weight range:	-
Synonyms:	-

Structural formula:

1.2 Similar substances/grouping possibilities

The chemical safety report provided by the registrant for esterification products of 1,3-dioxo-2-benzofuran-5-carboxylic acid with nonan-1-ol mostly is based on read-across by comparison with source substances (structural analogous components).

Structural formula:



R: mainly C9 alkyl substitutes, C9 linear alkyl rich

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

RMOA	☐ Risk Management Option Analysis (RMOA)	
REACH Processes	Evaluation	☐ Compliance check, Final decision
		☐ Testing proposal, Final decison
		☐ CoRAP and Substance Evaluation
	Authorisation	☐ Candidate List
		☐ Annex XIV
	Restri -ction	☐ Annex XVII[1]
Harmonised C&L	☐ Annex VI (CLP) (see section 3.1)	
Processes under other EU legislation	☐ Plant Protection Products Regulation Regulation (EC) No 1107/2009	
	☐ Biocidal Product Regulation Regulation (EU) 528/2012 and amendments	
Previous legislation	☐ Dangerous substances Directive Directive 67/548/EEC (NONS)	
	☐ Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS)	
(UNEP) Stockholm convention (POPs Protocol)	☐ Assessment	
	☐ In relevant Annex	

[1] Please specify the relevant entry.

Other processes / EU legislation	☐ Other (provide further details below)

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

There is no harmonised classification and there are no notified hazards by manufactures, importers or downstream users for this substance.

Brief summary of the hazard profile:

Human health

-Acute toxicity :
LD50 for oral acute toxicity = 2000-9850 mg/kg/pc (rat)
LD50 () 3200-60 000 mg/kg/pc (mouse). (read across with TOTM, trioctyl trimelittate and 1,2,4-Benzenetricarboxylic acid, decyl octyl ester).
LC50 for acute inhalation toxicity (4h) > 2600 mg/m3 (read across with TOTM).
LC50 for acute inhalation toxicity (6h) > 230 mg/m3 (read across with TOTM).
LD50 for acute dermal toxicity > 2000 mg/kg/pc (rat) avec TOTM.

LD50 for acute dermal toxicity > 2 ml/kg/pc (rabbit) avec le TM9.
LD50 for acute dermal toxicity > 20ml/kg/pc (guinea pig) avec TOTM.

-Repeated dose toxicity (Read across with structural analogous substances) :
Subacute toxicity :
TM8-10 (structural analogous) NOAEL=300 mg/kg/pc and LOAEL=1000 mg/kg/pc.
TM8 : NOEL=30 mg/kg/pc and LOAEL=125 mg/kg/pc.
Subchronic toxicity :
TM8-10 : NOAEL =500 mg/kg/j.
TOTM: NOAEL=225 mg/kg/j and LOAEL=1000 mg/kg/j.
-Skin and ocular irritation (Read across with structural analogous substances) :
Skin irritation / corrosion : no adverse effect observed (not irritating)
Eye irritation / corrosion : no adverse effect observed (not irritating)
-Skin sensitization (Read across with structural analogous substances) :
Not sensitizing.
-Mutagenicity (Read across with structural analogous substances) :
No evidence of genotoxicity in vitro and in vivo.
-Reproductive toxicity (Read across with structural analogous substances) :
-Carcinogenicity (Read across with structural analogous substances) :
No study available.

Environment:

The environmental fate and ecotoxicological hazard properties of esterification products of 1,3-dioxo-2-benzofuran-5-carboxylic acid with nonan-1-ol are based on read-across approach by comparison with hazard properties of structural analogous components which are not clearly determined regarding their hazard properties, and are only based on predictive data (QSAR).

Release to the environment of this substance is likely to occur from industrial use: in the production of articles and formulation of mixtures. Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials), indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment), indoor use, outdoor use resulting in inclusion into or onto a materials (e.g. binding agent in paints and coatings or adhesives), indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters) and outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids).

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[2]

4.1 Tonnage and registration status

Table: Tonnage and registration status

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
Joint submission		

4.2 Overview of uses

This substance is used in the following products: polymers, lubricants and greases.

This substance is used for the manufacture of: plastic products, machinery and vehicles, chemicals, rubber products and electrical, electronic and optical equipment.

Part 1:

☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☒ Consumer use	☒ Article service life	☐ Closed system

Part 2:

	Use(s)
Uses as intermediate	Not applicable
Formulation	The substance is used as a softener in the formulation of plastisol and as a lubricant additives in the formulation of lubricants and their

[2] *The dissemination site was accessed in April 2016 .*

	additives. The substance is also used as a softener in the formulation of substance with antioxidants.
Uses at industrial sites	The substance is used at industrial sites as softener in the manufacture of plastic products (pellets and dry-blend) and plastic articles. The substance is also used at industrial site as softeners in cable and car interior compoundings. The substance is used at industrial sites as a lubricant and lubricant additives in the manucfacture of bulk and large-scale chemicals (including petroleum products).
Uses by professional workers	The substance can be used as a lubricant and lubricant additive by professional workers (e.g manufacture of rubber and plastic products, manufacture of computer, electronic and optical products, electrical equipment and transport equipment). Professionals can use articles obtained by calendering, extrusion, slush moulding, injection moulding and blowing. They can also use articles obtained by spread coating, dipping, pouring, rotational molding, coil coating. In all theses articles used by professionals, the substance is used as a softener during the formulation.
Consumer Uses	Consumers can use lubricants and greases containing the substance. Consumers can use building materials and car interiors where the substance is used as a softerner.
Article service life	This substance can be used as a lubricant and lubricant additive in complex articles such as vehicles, machinery, mechanical appliances and electrical/electronic products (e.g. computers, cameras, lamps, refrigerators, washing machines). This substance can be used as a softener in electrical batteries and accumulators. This substance can be also found in products with material based on: plastic (e.g. food packaging and storage, toys, mobile phones).

Release to the environment of this substance is likely to occur from industrial use: in the production of articles and formulation of mixtures. Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials), indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment), indoor use, outdoor use resulting in inclusion into or onto a materials (e.g. binding agent in paints and coatings or adhesives), indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters) and outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids).

Part 3: There is high potential for exposure of

☐ Humans	☒ Environment

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

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 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[3]	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[1]	☐ Other (please specify below)
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)

[3] 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

A comparison of the physico-chemical, toxicological, environmental fate, and ecotoxicological parameters indicate that the validity of the read-across proposed in the dossier with other members of the trimellitates category to address various human health and environmental endpoints may be questionable. A prior CCH would confirm the identified concern and may conclude on the acceptability of the read-across. Additional toxicokinetic data may also be required under Substance Evaluation to clarify and substantiate it.

It appeared that there is also a concern for the PBT assessment of the substance, as described below.

One trimellitate TOTM may have ED effects which have been/are still evaluated by AT. Therefore there could be an ED concern for the TM9 if the read-across is acceptable.

When read-across will be stabilized, further evaluation will need to be carried out in particular for all these endpoints.

Human health:

Based on the information included in the dossier, a CCh is deemed necessary before the substance evaluation in order to evaluate the validity of the read-across proposed, and to address any potential data gaps which include at least carcinogenicity and reprotoxicity.

Concerning the reprotoxicity of Diplast TM9, no study performed with TM9 is available. There is a proposal for a read-across with a study performed with TOTM in which this substance exhibits a slight increase in retained areolar region in males at hight dosage on PND1. A reduced spermatocytes and spermatides in the testes of males was observed at doses of 300 or 1000 mg/kg/j without functional changes in fertility or reproductive performance. Therefore a concern exists for Diplast TM9 for reprotoxicity which needs to be further investigated.

Environmental hazards:

First, a prior CCH would confirm the identified concerns.

Based on the available information concerning the persistence, the bioaccumulation and the toxicity of the substance and its potential relevant metabolites in the environment, there are still uncertainties on the PBT/vPvB concern. It appears that the remaining concern is due to equivocal results relative to the estimated biodegradation, the estimated bioaccumulation factor for a substance which is outside of Log Kow range of the training set compounds and the estimated ecotoxicity data based on tests performed under equivocal conditions regarding the hazard properties of Diplast TM9 considered as a difficult substance (UVCB with low solubility, high Kow, high adsorption).

All the data are based on structural similarity with other trimellitates for which QSAR data are provided, or based on the estimated data for the major constituant trinonyl benzene-1,2,4-tricarboxylate (typical concentration 63.7%). Its structural similarity (that needs to be substantiated because they have differences in key parameters) with the TOTM underlines the theorical possibility that the metabolite mono (2-ethylhexyl)phthalate (MEHP), a major metabolite of DEHP, is formed as it was stated for TOTM. Whether metabolites occur in the different environmental compartments is not know based on the screening of the registration dossier. Then the potential degradation products of Diplast TM9 in environmental compartments have to be addressed for their potential ecotoxicity which might lead to the fulfillment of the T criterion but also for their potential persistence or bioaccumulation. Finally, the structural similarity of Diplast TM9 with TOTM and its potential similar/common metabolites to those of TOTM raised the question of the potential endocrine disruption property of Diplast TM9 and its metabolites.

In conclusion it is not possible to conclude on the PBT assessment of the substance, therefore a concern exists for the endpoint, because of the potential persistence of the

substance, since the bioaccumulation is still equivocal and toxicity needs to be further investigated.

Exposure assessment and risk characterisation have not been performed since the substance is currently not classified. But, based on the available data from the registration dossier and the dissemination site, since the substance is used for instance in lubricants and greases, coating products, fillers, putties, plasters, modelling clay, finger paints and hydraulic fluids and the concerns raised, a classification may be proposed following the evaluation of the substance. Thus, exposure assessment and risk characterisation should be investigated.

5.4 Preliminary indication of information that may need to be requested to clarify 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)

For human health, information may be need in order to clarify the concern for reprotoxicty of the substance and possible ED properties.
Information regarding fate and behavior, and ecotoxicity of the substances including degradation products are needed to conclude on the PBT/vPvB criteria and to justify that exposure and risk assessment are or are not needed.
More information are needed to investigate the ED potential for the environment because TM9 is an analogue to ToTM, that a read-across to this substance is proposed in the registration dossier and alert exists for the potential endocrine properties of this substance.

5.5 Potential follow-up and link to risk management

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

Identification of the substance as SVHC for ED or PBT properties