Substance Name: Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP) [with **≥0.1%** w/w 4-heptylphenol, branched and linear[1]]

EC Number: -

CAS Number: -

MEMBER STATE COMMITTEE

SUPPORT DOCUMENT

FOR IDENTIFICATION OF

REACTION PRODUCTS OF 1,3,4-THIADIAZOLIDINE-2,5-DITHIONE, FORMALDEHYDE AND 4-HEPTYLPHENOL, BRANCHED AND LINEAR[2] (RP-HP)

AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF THEIR ENDOCRINE DISRUPTING PROPERTIES WHICH CAUSE PROBABLE SERIOUS EFFECTS TO THE ENVIRONMENT WHICH GIVE RISE TO AN EQUIVALENT LEVEL OF CONCERN TO THOSE OF CMRs[3] AND PBTs/vPvB[4] SUBSTANCES (ARTICLE 57(F))

Adopted on 30 November 2017

[1] The full name of the entry 4-heptylphenol, branched and linear as it is included in the Candidate List is: 4-Heptylphenol, branched and linear *[substances with a linear and/or branched alkyl chain with a carbon number of 7 covalently bound predominantly in position 4 to phenol, covering also UVCB- and well-defined substances which include any of the individual isomers or a combination thereof]*

[2] The full name of the entry as it is proposed for the Candidate List is: Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP) [with ≥0.1% W/W 4-heptylphenol, branched and linear]

[3] CMR means carcinogenic, mutagenic or toxic for reproduction

[4] PBT means persistent, bioaccumulative and toxic; vPvB means very persistent and very bioaccumulative

CONTENTS

TABLES

ABBREVIATIONS

C&L	Classification & Labelling
dph	Days post hatch
GC/MS	Gas chromatography–mass spectrometry
4-HPbl	4-Heptylphenol, branched and linear
4nHP	4-n-Heptylphenol
IPCS	International Programme on Chemical Safety
LOD	Limit of detection
LOQ	Limit of quantification
OECD	Organisation for Economic Co-operation and Development
RP-HP	Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear
SVHC	Substance of very high concern
UVCB	Substances of Unknown or Variable composition, Complex reaction products or Biological materials
WHO	World Health Organization

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

Substance Name: Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP) [with ≥0.1% w/w 4-heptylphenol, branched and linear (4-HPbl)]

EC Number: -

CAS number: -

- The substances are identified as substances of equivalent level of concern to those of other substances listed in points (a) to (e) of Article 57 of Regulation (EC) No 1907/2006 (REACH) according to Article 57(f) of REACH Regulation.

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

Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear with ≥0.1% w/w of 4-heptylphenol, branched and linear, are identified as substances of very high concern in accordance with Article 57(f) of Regulation (EC) 1907/2006 (REACH), because they are substances with endocrine disrupting properties for which there is scientific evidence of probable serious effects to the environment which gives rise to an equivalent level of concern to those of other substances listed in points (a) to (e) of Article 57 REACH[5].

The Member State Committee at its 51st meeting unanimously agreed that 4-Heptylphenol, branched and linear *[substances with a linear and/or branched alkyl chain with a carbon number of 7 covalently bound predominantly in position 4 to phenol, covering also UVCB- and well-defined substances which include any of the individual isomers or a combination thereof]* meet the criteria set out in Article 57(f) of REACH. The reasoning is laid down in the "Member State Committee support document for identification of 4-heptylphenol, branched and linear (4-HPbl) as a substance of very high concern because of its endocrine disrupting properties which cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMR and PBT/vPvB substances", adopted on 14 December 2016[6]. ECHA has included 4-HPbl in the Candidate List for eventual inclusion in Annex XIV[7].

Therefore, reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP) with ≥0.1%[8] w/w 4-heptylphenol, branched and linear, are likewise identified as substances of very high concern due to their endocrine disrupting properties to the environment.

[5] https://echa.europa.eu/documents/10162/843b45f2-fc7d-5a41-a1fd-fda3adb4db59

[6] https://echa.europa.eu/documents/10162/f3dba6ab-8dd8-2457-4213-2f390b0539f1

[7] Decision of the European Chemicals Agency on the Inclusion of substances of very high concern in the Candidate List for eventual inclusion in Annex XIV: https://echa.europa.eu/documents/10162/0f8c5cf3-ccb7-3df6-c351-1c2df00cbc91

[8] Ref. to REACH, Article 56 (6)a.

Registration dossiers submitted for substances belonging to this group entry: Yes, for the substance identified by the registrant using the chemical name “reaction product of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and phenol, heptyl derivs.” It is noted that only one starting material consisting of 4-heptylphenol, branched and linear has been registered. This starting material has been identified by the registrant as “phenol, heptyl derivs.” (EC No. 276-743-1).

Justification

1. Identity of the substance and physical and chemical properties

1.1 Name and other identifiers of the substance

Table 1: Substance identity

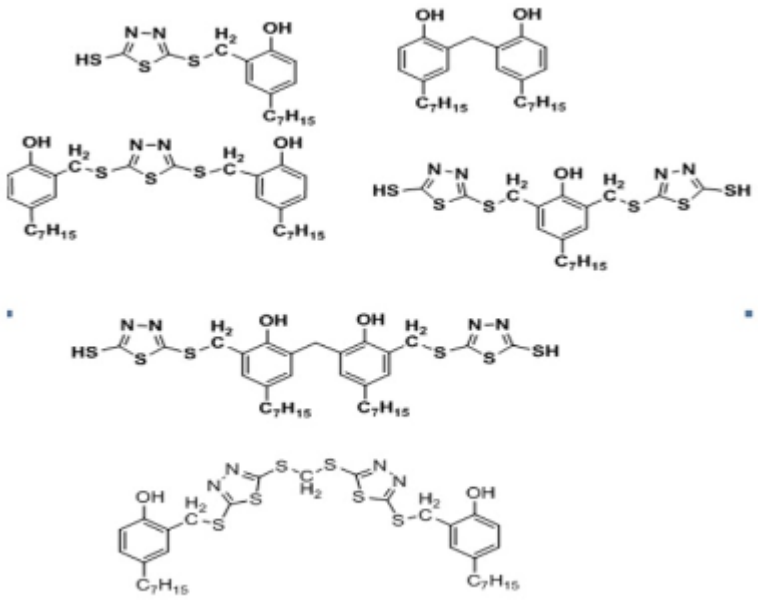
EC number:	-
EC name:	-
CAS number (in the EC inventory):	-
CAS number: Deleted CAS numbers:	-
CAS name:	-
IUPAC name:	Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear [with ≥0.1% w/w 4-heptylphenol, branched and linear]
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	-
Molecular weight range:	
Synonyms:	-

One of the substances belonging to this group has been registered. It has been identified using the chemical name “Reaction product of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and phenol, heptyl derivs.”. It is noted that before this registration the following chemical identifiers have been used instead: Formaldehyde, reaction products with branched and linear heptylphenol, carbon disulfide and hydrazine (EC No 300-298-5, CAS 93925-00-9). 1,3,4-thiadiazolidine-2,5-dithione can indeed be manufactured from carbon disulfide and hydrazine. Although currently not registered, the chemical identifier “formaldehyde, reaction products with branched and linear heptylphenol, carbon disulfide and hydrazine (EC No 300-298-5, CAS 93925-00-9) shall be covered by this proposal.

RP-HP may contain significant amount of process solvent (X) that cannot be removed without affecting the stability of the substance or changing its composition. In this situation, the presence of the solvent (X) may as a result be rightfully quoted in the name of the substance (for example, such substance can be named as “Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear including ‘solvent X’ ”). Such substance will still be covered by this proposed entry as long as it contains ≥0.1% w/w 4-heptylphenol, branched and linear. More generally, any variation in the composition resulting from the use of different processing agents/solvents and/or additives does not establish a criterion to exclude any substance resulting from the reaction between 1,3,4-thiadiazolidine-

2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear from the proposal.

Structural formula: idealised structure[9]



1.2 Composition of the substance

Name: Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear [with ≥0.1 % w/w 4-heptylphenol, branched and linear]

Description: group entry

Substance type: UVCB[10]

1.3 Identity and composition of degradation products / metabolites relevant for the SVHC assessment

Not applicable.

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

Not applicable.

1.5 Physicochemical properties

For the registered UVCB substance "reaction product of 1,3,4-thiadiazolidine-2,5-dithione,

[9] Source: ECHA dissemination site: https://echa.europa.eu/de/registration-dossier/-/registered-dossier/12316, accessed July 2017

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

formaldehyde and phenol, heptyl derivs.", which is covered by the group entry, physicochemical properties are given in Table 2 below.

Table 2: Overview of physicochemical properties

Property	Description of key information	Value [Unit]	Reference/source of information*
Physical state at 20°C and 101.3 kPa	The substance is an amber coloured liquid with no reported odour.	Liquid at 20°C and 1013 hPa	Dissemination site
Melting/freezing point	A melting point or melting range is not available for this UVCB substance. Two pour points are given in the registration dossiers depending probably on different methods and/or compositions of the measured UVCB substance.	Pour point: -3°C Pour point: 9 ± 3°C	Dissemination site
Boiling point	A boiling point or boiling range is not available, as substance decomposes.	Start of decomposition from 244°C at 1009 hPa	Dissemination site
Vapour pressure	According to EU Method A.4 (Vapour Pressure) Effusion method: vapour pressure balance	0.076 Pa	Dissemination site
Density	Test Guidance: ASTM D4052-09 Standard Test Method for Density and Relative Density of Liquids by Digital Density Meter	1.12 g/mL at 15.6°C	Dissemination site
Water solubility	OECD Guideline105 for Testing of Chemicals (flask method)	$\leq 1.14 \times 10^{-4}$ g/L at 20.0± 0.5°C.	Dissemination site
Partition coefficient n-octanol/water (log value)	OECD Guideline 117 (Partition Coefficient (n-octanol / water), HPLC Method)	The test substance is a mixture of components with logPow values ranging from 5.31 to 11.41	Dissemination site

*https://echa.europa.eu/information-on-chemicals/registered-substances. Dissemination site was accessed at 19.07.2016

2. Harmonised classification and labelling

No harmonised classification and labelling is available for any of the substances in the group of RP-HP.

Furthermore, no harmonised classification and labelling is available for any of the substances in the group of 4-Heptylphenol, branched and linear.

3. Environmental fate properties

The identification of RP-HP with ≥0.1% w/w 4-heptylphenol, branched and linear as substances of very high concern in accordance with Article 57(f) of Regulation (EC) 1907/2006 (REACH) is based on the identification of 4-heptylphenol, branched and linear (4-HPbl) as a group of substances with endocrine disrupting properties for which there is scientific evidence of probable serious effects to the environment which gives rise to an equivalent level of concern to those of other substances listed in points (a) to (e) of Article 57 REACH.

The group of 4-HPbl is already included in the candidate list. A detailed assessment of their environmental fate properties is available in the "Member state committee support document for identification of 4-heptylphenol, branched and linear (4-HPbl) as a substance of very high concern because of its endocrine disrupting properties which cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMR and PBT/vPvB substances", adopted on 14 December 2016[11].

A literature search for new scientific data on 4-HPbl has been performed in July 2017, however, no new data that would add to the assessment of endocrine disrupting properties of 4-HPbl have been identified.

4. Human health hazard assessment

See Chapter 3.

A detailed assessment of the human health hazards of 4-HPbl is available in the "Member state committee support document for identification of 4-heptylphenol, branched and linear (4-HPbl) as a substance of very high concern because of its endocrine disrupting properties which cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMR and PBT/vPvB substances", adopted on 14 December 2016[11].

A literature search for new scientific data on 4-HPbl has been performed in July 2017, however, no new data that would add to the assessment of endocrine disrupting properties of 4-HPbl have been identified.

5. Environmental hazard assessment

See Chapter 3.

A detailed assessment of the environmental health hazards of 4-HPbl is available in the "Member state committee support document for identification of 4-heptylphenol, branched and linear (4-HPbl) as a substance of very high concern because of its endocrine disrupting properties which cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMR and PBT/vPvB substances", adopted on 14 December 2016[11].

[11] https://echa.europa.eu/documents/10162/f3dba6ab-8dd8-2457-4213-2f390b0539f1

A literature search for new scientific data on 4-HPbl has been performed in July 2017, however, no new data that would add to the assessment of endocrine disrupting properties of 4-HPbl have been identified.

6. Conclusions on the SVHC Properties

6.1 CMR assessment

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (f) of REACH.

6.2 PBT and vPvB assessment

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (f) of REACH.

6.3 Assessment under Article 57(f)

Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear [with ≥0.1% w/w 4-heptylphenol, branched and linear] are identified as a substances of very high concern in accordance with Article 57(f) of Regulation (EC) 1907/2006 (REACH) where they contain any constituent or group of constituents (including impurities) of the group "4-heptylphenol, branched and linear" ≥0.1% in total owing to its endocrine disrupting properties for which there is scientific evidence of probable serious effects to the environment which gives rise to an equivalent level of concern to those of other substances listed in points (a) to (e) of Article 57 of REACH.

6.3.1 Conclusion on the hazard properties and equivalent level of concern assessment

Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear with ≥0.1% w/w of 4-heptylphenol, branched and linear, are identified as substances of very high concern in accordance with Article 57(f) of Regulation (EC) 1907/2006 (REACH), because they are substances with endocrine disrupting properties for which there is scientific evidence of probable serious effects to the environment which gives rise to an equivalent level of concern to those of other substances listed in points (a) to (e) of Article 57 REACH[12].

The Member State Committee at its 51st meeting unanimously agreed that 4-Heptylphenol, branched and linear *[substances with a linear and/or branched alkyl chain with a carbon number of 7 covalently bound predominantly in position 4 to phenol, covering also UVCB- and well-defined substances which include any of the individual isomers or a combination thereof]* meet the criteria set out in Article 57(f) of REACH. The reasoning is laid down in the "Member State Committee support document for identification of 4-heptylphenol, branched and linear (4-HPbl) as a substance of very high concern because of its endocrine disrupting properties which cause probable serious effects to the environment which give rise to an equivalent level of concern to those of CMR and PBT/vPvB substances", adopted on 14 December 2016[13]. ECHA has included 4-HPbl in the Candidate List for eventual inclusion in Annex XIV[14].

[12] https://echa.europa.eu/documents/10162/843b45f2-fc7d-5a41-a1fd-fda3adb4db59

[13] https://echa.europa.eu/documents/10162/f3dba6ab-8dd8-2457-4213-2f390b0539f1

Therefore, reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP) with ≥0.1%[15] w/w 4-heptylphenol, branched and linear, are likewise identified as substances of very high concern due to their endocrine disrupting properties to the environment.

[14] Decision of the European Chemicals Agency on the Inclusion of substances of very high concern in the Candidate List for eventual inclusion in Annex XIV: https://echa.europa.eu/documents/10162/0f8c5cf3-ccb7-3df6-c351-1c2df00cbc91

[15] Ref. to REACH, Article 56(6)a.