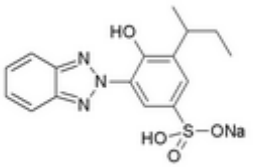
Justification Document for the Selection of a CoRAP Substance

EC/List number	CAS RN	Public Substance name	Chemical structure	Registration type (t/y) [1]
403-080-9	92484-48-5	Sodium 3-(2H-benzotriazol-2-yl)-5-sec-butyl-4-hydroxybenzenesulfonate		≥ 10 Full

Authority: Spanish Ministry for the Ecological Transition

Date: 21 March 2023

Revision history

Version	Date

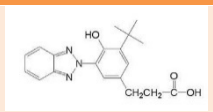
Cover Note

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

[1] Note that the total aggregated tonnage band may be available on ECHA's webpage at https://echa.europa.eu/information-on-chemicals/registered-substances

1. Background

1.1 Analogue substances

EC/List number	CAS RN	Public Substance name	Chemical structure	Registration type (t/y)
630-348-4	84268-36-0	Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-		Intermediate

Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy- (EC 630-348-4), referred to as metabolite M1 is similar to the free acid form of the substance covered in this JD, only differing in the acid group (propionic acid instead of sulfonic acid) and in the branching of the butyl substitution group. The presence of the -SO3H group increases water solubility due to its ability to act as both a H-bond donor and acceptor.

1.2 Overview of ongoing / completed / other processes & other EU legislation

EC/ List number	Evaluation			CLH	Restriction	Authorisation
	CCH	TPE	Previously on CoRAP	Annex VI (CLP)	Annex XVII*	Candidate List/ Annex XIV
403-080-9	-	-	-	Index no. 613-095-00-4	-	-

**Some of the broad restriction entries in the Annex XVII of REACH are not represented in the overview, e.g. when the scope of the restriction is defined by its classification or the substance identification is broad (e.g. entries 3, 28-30 and 40)*

EC/ List number	Other EU legislation	Previous legislation	Stockholm convention	Other
	PPP/ BPR	NONS/ RAR	POP	(e.g. UNEP)
403-080-9	-	-	-	-

2. Classification

You can find information on classification in the ECHA C&L Inventory database, which includes both harmonised classification (when available) and the notified self-classifications. (http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database].
The CLP Regulation and all published ATPs are available on ECHA website: http://echa.europa.eu/web/guest/regulations/clp/legislation .

EC/ List No	CAS RN	Public Substance name	Harmonised classification	Classification in registrations	Classification in C&L notifications (*)
403-080-9	92484-48-5	Sodium 3-(2H-benzotriazol-2-yl)-5-sec-butyl-4-hydroxybenzenesulfonate	Eye Dam. 1, H318	Eye Dam. 1, H318 Aq. Chronic 3, H412	H318 (175) H412 (88)

(*) the number in brackets indicates the number of notifications received. Each notification can represent a group of notifiers. Therefore the number may differ from the C&L inventory which displays number of notifiers.

3. Tonnage and uses

3.1 Aggregated Tonnage

EC/ List No	Aggregated tonnage (as per ECHA dissemination website)*
403-080-9	≥ 10 t/y

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

3.2 Overview of the Uses

Main types of applications	EC 403-080-9 Key information
Manufacture	Chemical production or refinery where opportunity for exposure arises
Formulation	Used in the chemical production with occasional controlled exposure arises
Industrial use	Used as a processing aid in textiles, industrial chemical processes, charging and discharging of substances and mixtures, in cleaning agents, as intermediate and in laboratories as a laboratory reagent.
Professional use	Used as processing aid in textiles and cleaning agents

Consumer Use	Exposure and releases are expected from consumer widespread uses in perfumes and fragrances, cosmetic and personal care products and washing and cleaning products
Article service life	Use in cleaning agents
Intermediate use (if TII)	

This substance is used in perfumes and fragrances, washing & cleaning products and cosmetics and personal care products. The substance is mainly used as a light stabiliser in cosmetics.

Release to the environment can occur from industrial use at industrial sites: manufacturing of the substance and in processing aids, formulation of mixtures, in the production of articles, as an intermediate step in further manufacturing of another substance (use of intermediates) as processing and the manufacture of: textile, leather or fur.

Other release to the environment of this substance is likely to occur from consumer uses, article service life: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners) and outdoor use.

ECHA has no public registered data indicating whether or into which articles the substance might have been processed or used.

4. Justification for inclusion on the CoRAP

4.1 Legal basis

☒ Article 44(2)[2]

☐ Article 45(5)[3]

4.2 Identification of initial grounds of concern

Hazard-based concerns	
Suspected CMR	☐ Carcinogenic ☐ Mutagenic ☐ Reproductive toxicant
Potential ED	☐ Human Health ☐ Environment

[2] "The Agency shall use the criteria in paragraph 1 […]. Substances shall be included if there are grounds for considering (either on the basis of a dossier evaluation carried out by the Agency or on the basis of any other appropriate source, including information in the registration dossier) that a given substance constitutes a risk to human health or the environment."

[3] "A Member State may notify the Agency at any time of a substance not on the Community rolling action plan, whenever it is in possession of information which suggests that the substance is a priority for evaluation. […]".

Suspected Sensitiser	☐ Respiratory ☐ Skin
Specific target organ toxicity – repeated (STOT RE)	☐ (as defined in section 4.3 below)
Suspected PBT/ vPvB Suspected PMT/ vPvM	☐ Persistent ☐ Bioaccumulative ☐ Mobile ☐ Toxic (as defined in section 4.3 below) ☒ very Persistent ☐ very Bioaccumulative ☒ very Mobile
Other human health hazard(s)	☐ (as defined in section 4.3 below)
Other environmental hazard(s)	☒ (as defined in section 4.3 below)
Exposure / risk-based concerns	
Wide dispersive use	☒
Consumer use	☒
Exposure of workers	☐
Exposure of sensitive populations	☐
Exposure of environment	☒
Cumulative exposure	☒
High RCR	☐
High (aggregated) tonnages	☐
Others: Exposure of water reservoirs and drinking water.	☒

4.3 Justification of the concern(s) – to be clarified under Substance evaluation

Existing data supporting the hazard-based concern

The substance Sodium 3-(2H-benzotriazol-2-yl)-5-sec-butyl-4-hydroxybenzenesulfonate is a multiconstituent substance.

Persistency

The hydrolytic stability of sodium 3(2H-benzotriazol-2-yl)-5-sec-butyl-4-hydroxybenzenesulfonate tested according to OECD 111, resulted in a half-life of more than 1 year at 25 °C and pH 4, 7 and 9.

The results of the BIOWIN QSAR models 2, 3 and 6 indicate that the free acid form of the substance should be considered as a borderline case for meeting the screening criteria for P/vP included in ECHA Guidance R.11. Based on the CATALOGIC 301c QSAR model prediction the acid form of the substance is likely to be persistent.

In a test conducted according to the OECD guideline 301A, 0 % biodegradation was observed after 28 days. The test item is therefore evaluated as not readily biodegradable. No inhibition on the activity of the bacteria was found at the test substance concentration of 40 mg/L.

No simulation studies are available for the substance.

Therefore, based on the available information the substance screens as P/vP.

Mobility

The substance has a high water solubility (9.8 g/L). Based on the provided physicochemical properties (MW: 370.385; VP: $6.06*10^{-18}$ Pa at 20°C; log Pow of -0.24 (25°C)), EUSES estimated a log Koc of 0.74.

The dissociation of test substance was determined to be pKa = 7.93 at 25°C. The European Commission's draft proposal is that for ionisable substances a log Koc < 2 at pH 4-9 would be sufficient to conclude as very mobile (vM).

The log Kow method in KOCWIN predicts log Koc values of 0.86 and 1.85 when entering the SMILES of the salt form and acid form, respectively. This difference is caused by the fact that the log Kow predicted by KOWWIN for the salt form is actually for the ionised acid form whereas the log Kow predicted for the acid form is for the neutral form of the acid. It is noted that the KOCWIN log Kow method model recognises sulfonic acid fragment and the correction factor for this fragment is 0.00. It is not clear whether this refers to the acid group in ionised or neutral form.

It is noted that as the substance is ionisable the log Koc values are expected to vary with pH. Furthermore, different ionic interactions may lead to sorption in soils and sediments, and these are difficult to predict.

Therefore, based on the available information the substance screens as M/vM with a log Koc <2.

Toxicity

No data available on long-term effects on fish. ECOSAR predicts low chronic toxicity in fish (ChV values 123-206 mg/L for baseline toxicity, benzotriazoles-acid and phenols-acid classes).

Based on the available data not possible to conclude on toxicity, likely not-T but it needs to be confirmed.

Other relevant information to justify the inclusion in CoRAP

Information to be potentially requested

Request a simulation test (OECD 307, 308 and/or 309 to be decided) to clarify P/vP, request leaching in soil columns (OECD 312) to clarify on M/vM. Long-term aquatic toxicity tests to conclude on T.

***Possible follow-up** (demonstrating the improvement of risk management measures)*

EC/ List number	Harmonised C&L	Restriction	Authorisation	Other
403-080-9	☒	☐	☒	☐

If vPvM is confirmed a proposal for harmonized classification based on the new hazard classes of the CLP Regulation, once in force, could be prepared. Potential SVHC identification should be considered.