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SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate

EC No 404-800-4

CAS No 118832-72-7

Evaluating Member State(s): Germany

Dated: 3 March 2016

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Evaluating Member State Competent Authority

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Year of evaluation in CoRAP: 2014

The substance evaluation was terminated without requesting further information from the registrant under an Article 46(1) decision due to change in status of the registration dossier (cease manufacture in accordance with Article 50(3) of the REACH Regulation).

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

Iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate was originally selected for substance evaluation in order to clarify suspected concerns about:

- PBT (Persistent, Bioaccumulative and Toxic)

- vPvB (very Persistent and very Bioaccumulative)

During the evaluation, an additional concern related to the environmental release estimation of the substance was identified.

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

None

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State to the following conclusions, as summarised in the table below.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION Conclusions	Tick box
Need for follow-up regulatory action at EU level *[if a specific regulatory action is already identified then, please, select one or more of the specific follow-up actions mentioned below]*	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	X

The evaluating Member State Competent Authority (eMSCA) initially concluded that further information will be required to clarify the concerns regarding potential PBT/vPvB properties of the substance.

However, after receiving the substance evaluation draft decision, the only remaining registrant ceased manufacture of the substance in accordance with Article 50(3) and therefore revoked the registration. As there were no remaining active registrations, the substance evaluation was terminated.

Due to the termination of the substance evaluation decision making process, the requested information to clarify the concern was not delivered. Therefore, in opinion of

the eMSCA, the concern for potential PBT/vPvB properties of the substance remains unclear.

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

Table 2

REASON FOR REMOVED CONCERN The concern could be removed because	Tick box
Clarification of hazard properties/exposure	
Actions by the registrants to ensure safety, as reflected in the registration dossiers (cease of manufacture)	X

During the decision making process of substance evaluation, the only remaining registrant of the substance ceased its manufacture in accordance with Article 50(3) and substance evaluation was terminated. As there was no remaining use of the substance within the scope of substance evaluation, the concern was removed. At the time this report was finalised, there were no other active registrations for the substance.

The eMSCA recommends that further assessment of the potential PBT/vPvB hazard should be reinitiated in case of new registration of the substance in future.

5.2. Other actions

Not applicable.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

7.1. Overview of the substance evaluation performed

Iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate was originally selected for substance evaluation in order to clarify suspected concerns about:

- PBT (Persistent, Bioaccumulative and Toxic)

- vPvB (very Persistent and very Bioaccumulative)

During the evaluation, an additional concern related to the environmental release estimation was identified.

Table 3

EVALUATED ENDPOINTS Endpoint evaluated	Outcome/conclusion
Persistence	*The evaluating MSCA concluded that further information will be required to clarify the concern regarding persistence.* *However, due to termination of the substance evaluation process, no additional information was requested.*
Bioaccumulation	*The evaluating MSCA concluded that further information will be required to clarify the concern regarding bioaccumulation.* *However, due to termination of the substance evaluation process, no additional information was requested.*
Toxicity	*The evaluating MSCA concluded that further information will be required to clarify the concern regarding toxicity.* *However, due to termination of the substance evaluation process, no additional information was requested.*
Release estimation	*The evaluating MSCA concluded that further information will be required to clarify the concern regarding release estimation.* *However, due to termination of the substance evaluation process, no additional information was requested.*

7.2. Procedure

Pursuant to Article 44(2) of the REACH Regulation, Iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate was included on the Community rolling action plan (CoRAP) for evaluation in 2014. The Competent Authority of Germany was appointed to carry out the evaluation. The substance evaluation commenced on 26 March 2014.

The evaluation was targeted at environmental hazards and exposure.

The main source of information for the evaluation was the registration dossier.

Based on the evaluation of the available data, the evaluating MSCA concluded that there was a need to request further information to clarify the concerns regarding suspected PBT/vPvB as well as exposure, and therefore pursuant to Article 46(1) of the REACH Regulation prepared a draft decision to request further information. The draft decision was submitted to ECHA on 25 March 2015.

On the 06 May 2015, ECHA sent the draft decision to the registrant and invited them to comment by 11 Juni 2015. By that date, ECHA received comments from the registrant and forwarded them to the evaluating MSCA. On 15 July 2015, the registrant informed ECHA of their intention to cease manufacture in accordance with Article 50(3) of the REACH Regulation. ECHA informed the registrant about consequences and the registration of the substance was revoked on 4 August 2015. As there were no further registrants of the substance at that time, the substance evaluation decision making process was terminated without a decision requesting further information.

7.3. Identity of the substance

Table 4

SUBSTANCE IDENTITY	
Public name:	iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate
EC number:	404-800-4
CAS number:	118832-72-7
Index number in Annex VI of the CLP Regulation:	607-261-00-5
Molecular formula:	$C_{27}H_{46}O_3S$ to $C_{31}H_{54}O_3S$
Molecular weight range:	450.72 – 506.82 g/mol
Synonyms:	IRGANOX L 118

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

Structural formula:

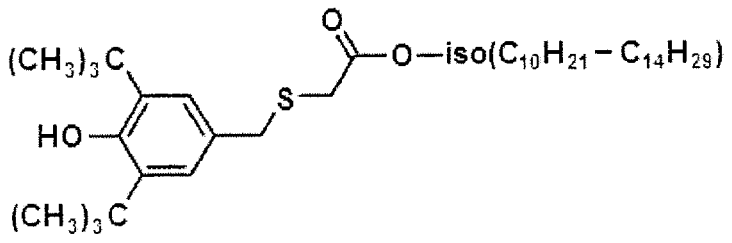

Table 5

Constituent

Name and EC number	Typical concentration	Concentration range	Remarks
iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl) methylthioacetate (respectively: C10-14 (branched) alkyl (3,5-di-tert-butyl-4-hydroxyphenyl) methylthioacetate) *EC number: 404-800-4*			For further Information, please see confidential Annex or rather IUCLID File.
Acetic acid dimethylamide [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-methyl]thiol]-			For further Information, please see confidential Annex or rather IUCLID File.
isotridecan-1-ol EC no.: 248-469-2			For further Information, please see confidential Annex or rather IUCLID File.
2,6-di-tert-butyl-α-dimethylamino-p-cresol EC no.: 201-816-1			For further Information, please see confidential Annex or rather IUCLID File.
Thioglycolic acid isotridecyl ester			For further Information, please see confidential Annex or rather IUCLID File.
2,6-di-tert-butylphenol EC no: 204-884-0			For further Information, please see confidential Annex or rather IUCLID File.
Dithioglycolic acid bis(isotridecyl ester)			For further Information, please see confidential Annex or rather IUCLID File.
2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol EC no: 204-279-1			For further Information, please see confidential Annex or rather IUCLID File.
Dimethylamine EC no: 204-697-4			For further Information, please see

			confidential Annex or rather IUCLID File.
(3,5-Di-tert-butyl-4-hydroxyphenyl)methylthioacetic acid			For further Information, please see confidential Annex or rather IUCLID File.
3,5-di-tert-butyl-4-hydroxybenzaldehyde EC no: 216-592-0			For further Information, please see confidential Annex or rather IUCLID File.

7.4. Physico-chemical properties

Table 6

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Value**
Physical state at 20°C and 101.3 kPa	yellowish viscous liquid
Vapour pressure	0.000036 Pa at 20°C 0.000068 Pa at 25°C Thermogravimetry
Surface tension	61.5 – 63.8 mN/m at 20°C (Filtrate of a 10.0068 g/L oil/water emulsion) Plate method
Water solubility	< 0.00008 g/L at 20°C at pH 6.6 flask method
Partition coefficient n-octanol/water (Log K_{ow})	logP_{ow}= 11.6 The calculation was based on Hansch-Leo Method using computer program CLOGP 3.4. The calculation was based on fragment method.
Stability in organic solvents and identity of relevant degradation products	The stability of the test substance is not considered to be critical.
Dissociation constant	pK_a= 12 at 25°C (calculated) The estimation was based scientific authoritative method.
Viscosity	1440-1470 mPa.s at 20°C

	200-210 mPa.s at 40°C The viscosity was measured by rotational viscometer.

7.5. Manufacture and uses

7.5.1. Quantities

At the beginning of the substance evaluation process, the tonnage was reported to be > 10 tonnes per annum. However, during the substance evaluation decision making process the two registrants ceased manufacture of the substance in accordance with Article 50(3) of the REACH Regulation and therefore the registration was revoked.

At the time of finalising this report, there were no active registrations within the scope of substance evaluation.

Table 7

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 - 10 t	x 10 - 100 t	☐ 100 - 1000 t	☐ 1000- 10,000 t	☐ 10,000-50,000 t
☐ 50,000 - 100,000 t	☐ 100,000 - 500,000 t	☐ 500,000 - 1000,000 t	☐ > 1000,000 t	☐ Confidential

7.5.2. Overview of uses

Table 8 At the start of the substance evaluation process, the uses listed below were identified. However, during the substance evaluation decision making process the registration was revoked in accordance with Article 50(3) of the REACH Regulation due to cease of manufacture. At the time of finalising this report, there were no active registrations for this substance.

USES Use(s)	
Uses as intermediate	None identified in the registration dossier
Formulation	Formulation of lubricants, greases, release products, hydraulic fluids, metal working fluids Formualtion of intermediate
Uses at industrial sites	Used in lubricants, greases, release products, hydraulic fluids, metal working fluids Used as intermediate
Uses by professional workers	Used in lubricants, greases, release products, hydraulic fluids, metal working fluids
Consumer Uses	Used in lubricants, greases, release products
Article service life	None identified in the registration dossier

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

Table 9

HARMONISED CLASSIFICATION ACCORDING TO ANNEX VI OF CLP REGULATION (REGULATION (EC) 1272/2008)							
Index No	International Chemical Identification	EC No	CAS No	Classification		Spec. Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)		
607-261-00-5	iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl)methylthioacetate	404-800-4	118832-72-7	Aquatic Acute 1 Aquatic Chronic 1	H400 H410		

7.6.2. Self-classification

No relevant information available.

7.7. Environmental fate properties

7.7.1. Degradation

Hydrolysis

The hydrolysis test could not be performed. Due to the low water solubility of Irganox L118 (< 0.08 mg/L) no analytical method with such a low detection limit could be developed ([redacted]).

Biodegradation in water

There are two screening tests on biodegradation available. As stated by the registrants, both key studies on biodegradation are GLP conform.

Ready biodegradation of Irganox L118 was measured according to OECD Guideline 301 B, Ready Biodegradability: CO_2 Evolution Test ([redacted]): (0% CO_2 Evolution after 28 days).

The chemical oxygen demand of Irganox L118 was determined according to DIN 38409 ([redacted]). A COD of 2.55 g COD/g test substance was calculated. Irganox L118 is not readily biodegradable.

7.7.2. Environmental distribution

Adsorption

The adsorption of Irganox L118 was determined according to OECD 121 guideline using the HPLC method ([redacted]). The log K_{oc} was estimated to be > 5.6 at 40°C (K_{oc} > 398107).

7.7.3. Bioaccumulation

No bioaccumulation study and no experimental log P_{ow} is available. The estimated log P_{ow} for Irganox L118 is 11.6 (no documentation according to Annex 11, CLOGP 3.4). Calculations in order to determine this log P_{ow} for Irganox L118 were done for C13 isomer. Based on the log P_{ow} of 11.6, the registrants has calculated three BCF values: 7.29 (CATALOGIC v5.11.2) [redacted], 34.69 (EPA T.E.S.T. v4.0.1) [redacted] and 211.00 (EPI Suite v4.10) [redacted]

7.8. Environmental hazard assessment

Some short- and long-term toxicity studies on different aquatic organisms for Irganox L118 have been provided in the registration dossiers. According to a long-term toxicity study on *Daphnia magna*, the UVCB substance is chronically toxic (NOEC (21d) = 0.00028 mg/L). No data regarding the toxicity potential of the single constituents of Irganox L118 including the alkyl chain constituents (C10-C14) is included in the registration dossiers.

7.8.1. Aquatic compartment (including sediment)

Fish

The acute toxicity to fish was assessed according to OECD guideline 203. In this 96-hour static acute toxicity test with zebrafish, the LC_{50} value was > 74.0 mg/L based on average measured concentrations ([redacted]). No mortality occurred during the test.

Aquatic invertebrates

The acute toxicity to invertebrates was assessed according to OECD guideline 202. In this 24-hour static toxicity test with *Daphnia magna*, the EC_{50} value was 1.3 mg/L (nominal concentration) ([redacted]).

The long-term toxicity to *Daphnia magna* was assessed according to OECD 211 ([redacted]). The NOEC for length of time for appearance of first brood was 0.00028 mg/L. The NOEC for the total cumulative number of young daphnia was 0.00028 mg/L, the NOEC for fraction of cumulative dead was 0.28 mg/L. The EC for immobilization was > 0.28 mg/L, the respective NOEC was 0.0045 mg/L.

Algae and aquatic plants

The toxicity to *Desmodesmus subspicatus* was assessed according to EEC directive 87/302/EEC ([redacted]). The respective NOEC was <0.16 mg/L, based on biomass.

7.8.2. Terrestrial compartment

7.8.3. Microbiological activity in sewage treatment systems

7.8.4. PNEC derivation and other hazard conclusions

7.8.5. Conclusions for classification and labelling

7.9. Human Health hazard assessment

Not evaluated.

7.10. Assessment of endocrine disrupting (ED) properties

Not evaluated.

7.11. PBT and vPvB assessment

Persistence

No data on hydrolysis is available. Due to the low water solubility of Irganox L118 (<0.08 mg/L) no analytical method with such a low detection limit could be developed. Irganox L118 is not readily biodegradable as shown by a screening test. No mineralisation was detected within 28 days.

In conclusion, Irganox L118 is considered to fulfil the screening criterion for persistency. However, no simulation tests on biodegradation in environmental compartments are available. Further testing on biodegradability is required to conclude whether Irganox L118 is persistent or very persistent according to REACH Annex XIII.

Bioaccumulation

The estimated log P_{ow} of 11.6 for Irganox L118 exceeds the screening criteria (log P_{ow} > 4.5) and therefore indicates a high potential for bioaccumulation. No measured bioaccumulation data is available. A final assessment whether Irganox L118 is bioaccumulative or very bioaccumulative according to REACH Annex XIII is not possible.

Toxicity

According to a long-term study on *Daphnia magna*, the UVCB substance is chronically toxic (NOEC (21 d) = 0.00028 mg/L) and therefore, fulfills the T-criterion according to REACH Annex XIII. No data on toxicity of the single constituents of the UVCB substance, including the different C10-C14 alkyl chain constituents, are available. Further testing on toxicity is required to conclude which constituent of Irganox L118 is toxic.

Overall conclusion

Based on the available data, final conclusions about the P/vP- and B/vB-criteria are not possible.

7.12. Exposure assessment

7.12.1. Human health

Not evaluated.

7.12.2. Environment

One full registration (two registrants in a joint submission) -existed for Irganox L118 in the tonnage band 10-100 t/a (ECHA dissemination site, 2014). Moreover, the substance has been notified as new substance under Directive 67/548/EEC (NONS).

According to the NONS information, the substance is mainly used as lubricant additive, i.e. antioxidant. In the registration dossiers, exposure scenarios have been mainly developed for industrial, professional and consumer use of lubricants and greases in vehicles or machinery as well as industrial, professional and consumer use in open systems. Lubricants containing Irganox L 118 are also used in industrial and professional high energy open processes.

Information has been provided on the manufacture of the substance and twelve different uses as shown in the table below.

Table 10 At the start of the substance evaluation process, the uses listed below were identified. However, during the substance evaluation decision making process the registration was revoked in accordance with Article 50(3) of the REACH Regulation due to cease of manufacture. At the time of finalising this report, there were no active registrations for this substance

MANUFACTURE AND USES OF IRGANOX L118 Manufacture and Uses	Environmental release category
Manufacture of lubricants and lubricant additives 1	ERC 1
Industrial formulation of lubricant additives, lubricants and greases. Includes material transfers, mixing, large and small scale packing, sampling, maintenance and associated laboratory activities. (ATIEL-ATC A)	ERC 2, 6A
General industrial use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines) (ATIEL-ATC B)	ERC 4, 7
General professional use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines) (ATIEL-ATC B)	ERC 9A, 9B
General consumer use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines) (ATIEL-ATC B)	ERC 9A, 9B
(Industrial) Use in open system. Application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways (ATIEL-ATC C)	ERC 4
(Professional) Use in open system. Application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion	ERC 8A, 8D

protection, slideways (ATIEL-ATC C)	

(Consumer) Use in open system. Application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways (ATIEL-ATC C)	ERC 8A, 8D
(Industrial) Use of lubricants in open high temperature processes, e.g. quenching fluids, glass release agents (ATIEL-ATC D)	ERC 4
(Industrial) Handling and dilution of metalworking fluid concentrates (ATIEL-ATC E)	ERC 2
(Industrial) Use of lubricants in high energy open processes, e.g. in high speed machinery such as metal rolling / forming or metalworking fluids for machining and grinding (ATIEL-ATC F)	ERC 4
(Professional) Use of lubricants in high energy open processes, e.g. in high speed machinery such as metal rolling / forming or metalworking fluids for machining and grinding (ATIEL-ATC F)	ERC 8a

Different types of spERCs have been assigned by the registrants. The underlying emission factors deviate from each other are considerably lower than the ERC according to ECHA Guidance R. 16 [The German Federal Environment Agency has examined selected spERCs in two research projects concluding that information on operational conditions in the spERC factsheets is often insufficient. Among others, it has been identified that ATIEL spERCs are not intended for the direct use by registrants and that emission estimation using these spERCs is not appropriate.]. Since the Chemical Safety Reports are lacking sufficient justification for the spERCs used, it is not clear whether operational conditions and applied risk management measures are covered by the selected spERCs. This leads to the concern that the assumptions do not necessarily reflect the worst case. Moreover, the waste stage has not been explicitly considered for any of the identified uses.

Due to the above-mentioned shortcomings, it is not possible to conclude on possible risks for the environment from manufacture and uses of Irganox L118. However, no further clarification was asked due to the cease of manufacture.

Aquatic compartment (incl. sediment)

Terrestrial compartment

Atmospheric compartment

7.12.3. Combined exposure assessment

7.13. Risk characterisation

7.14. References

Registration dossier for iso(C10-C14)alkyl (3,5-di-tert-butyl-4-hydroxyphenyl) methylthioacetate, European Chemicals Agency, http://echa.europa.eu/

7.15. Abbreviations

BCF	Bioconcentration factor
CAS	Chemical abstracts service
C&L	Classification and labelling
CLP	Classification, labelling and packaging (Regulation (EC) No 1272/2008)
EC_{50}	Effective concentration (50 %)
ERC	Environmental release concentration
LC_{50}	Median lethal dose

Log P_{ow}	*n*-octanol – water partitioning coefficient
MSCA	Member state competent authority
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative, Toxic
spERC	Special environmental release category
TG	Test guideline
TL	Testing laboratory
vPvB	Very Persistent and very Bioaccumulative