

**Substance Name: 2-ethylhexyl 10-ethyl-4,4-dioctyl-
7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
(DOTE)**

EC Number: 239-622-4

CAS Number: 15571-58-1

MEMBER STATE COMMITTEE

SUPPORT DOCUMENT FOR IDENTIFICATION OF

**2-ETHYLHEXYL 10-ETHYL-4,4-DIOCTYL-7-OXO-8-
OXA-3,5-DITHIA-4-STANNATETRADECANOATE
(DOTE)**

**AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE
OF ITS CMR¹ PROPERTIES**

Adopted on 9 December 2014

¹CMR means carcinogenic, mutagenic or toxic for reproduction

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ABBREVIATIONS

CAS	Chemical Abstract Service
CMR	Carcinogenic, Mutagenic or Toxic for reproduction
DOT	Diocetyltn
DOTE	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetra-decanoate
ECHA	European Chemicals Agency
IUPAC	International Unit of Pure and Applied Chemistry
MAK	Maximale Arbeitsplatzkonzentration
MOT	Monooctyltin
MOTE	2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
MSC	Member State Committee
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemical substances
SVHC	Substances of Very High Concern
vPvB	very Persistent and very Bioaccumulative

Substance Name: 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (DOTE)

EC Number: 239-622-4

CAS number: 15571-58-1

- 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (DOTE) is identified as substance meeting the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to its classification as toxic for reproduction category 1B.

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

Pursuant to Annex III of Commission Regulation (EU) No 944/2013 as of 2 October 2013 DOTE will be listed in Table 3.1 (List of harmonised classification and labelling of hazardous substances) of Annex VI, part 3, of Regulation (EC) No 1272/2008 as toxic for reproduction Repr. 1B, H360D (May damage the unborn child).

Therefore, this classification of DOTE in Commission Regulation (EC) No 944/2013 shows that the substance meets the criteria for classification in the hazard class:

- Reproductive toxicity category 1B in accordance with Article 57 (c) of REACH.

Registration dossiers submitted for the substance: YES

Justification

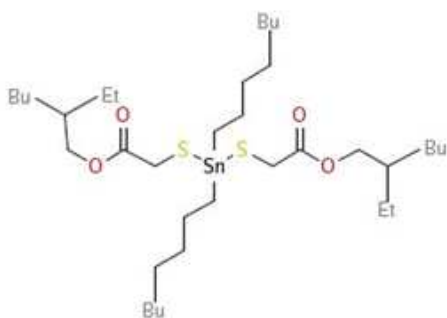
1. Identity of the substance and physical and chemical properties

1.1. Name and other identifiers of the substance

Table 1: Substance identity

EC number:	239-622-4
EC name:	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
CAS number (in the EC inventory):	15571-58-1
CAS number:	15571-58-1 CAS numbers deleted: 52433-96-2 64685-79-6 71061-19-3 85873-44-5
CAS name:	8-Oxa-3,5-dithia-4-stannatetradecanoic acid, 10-ethyl-4,4-dioctyl-7-oxo-, 2-ethylhexyl ester
IUPAC name:	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
Index number to be used in Annex VI of the CLP Regulation	050-027-00-7
Molecular formula:	C ₃₆ H ₇₂ O ₄ S ₂ Sn
Molecular weight range:	751.79
Synonyms:	DOTE, DOT(EHMA) ₂ , Dioctyltin bis(2-ethylhexyl mercaptoacetate), Dioctyltin bis(2-ethylhexyl) mercaptoacetate, Advastab 17MOL, 17MOK, Advastab 17 MOK, Acetic acid, 2,2'-((dioctylstannylene)-bis(thio))bis-, di-2-ethylhexyl ester, Bis(2-ethylhexyl thioglycolato)dioctyltin, Bis(2-ethylhexyl) ((dioctylstannylene)dithio)diacetate, Bis(carboxymethylthio)dioctylstannylene, di(2-ethylhexyl) ester, Di-n-octyltin bis(2-ethylhexyl mercaptoacetate), Di-n-octyltin-dithioglycolic acid 2-ethylhexyl ester, Dioctyltin bis(2-ethylhexyl thioglycolate), Dioctyltin bis(2-ethylhexylmercaptoacetate)

Structural formula:



It is noted that DOTE contains chiral carbon atoms in the ethylhexyl residue of the acetic ester group. The indicated CAS number does not reflect any specific stereoisomeric forms. No specification on the stereoisomers of DOTE is provided in the registrations. The SVHC dossier covers the substance including all possible stereoisomers.

1.2. Composition of the substance

Name: 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (DOTE)

Description: Well-defined substance comprising DOTE, including all possible stereoisomers, as main constituents

Degree of purity: See confidential Annex II (not included here)

DOTE is present in a reaction mass (multi-constituent substance), with the corresponding mono-octyltin (MOT) compound 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (MOTE) (CAS number: 27107-89-7, EC number: 248-227-6). The concentration ratio between DOTE and MOT in the reaction mass can differ depending on the manufacture of the mixture and the technical needs. The registrants have made use of the option allowing the registration of individual constituents for multi-constituent substances and have submitted registration dossiers for DOTE and MOT as individual substances. DOTE is the toxicologically relevant substance of concern and the DOTE registration contains all relevant exposure scenarios (taking pure DOTE as a generic worst case). Therefore, the present Annex XV SVHC dossier is submitted for the substance DOTE. In addition, a separate Annex XV SVHC dossier is submitted for the reaction mass DOTE:MOTE.

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

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

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

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

1.5. Physicochemical properties

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

2. Harmonised classification and labelling

Pursuant to Annex III of Commission Regulation (EU) No 944/2013² of 2 October 2013 DOTE will be listed in Table 3.1 (List of harmonised classification and labelling of hazardous substances) of Annex VI, part 3, of Regulation (EC) No 1272/2008³ as toxic for reproduction Repr. 1B, H360D (May damage the unborn child).

Therefore, this classification of the substance in Commission Regulation (EC) No 944/2013 shows that the substance meets the criteria for classification as toxic for reproduction in accordance with Article 57 (c) of REACH.

Table 2: Harmonised classification according to Regulation (EC) No 944/2013

Index No	International Chemical Identification	EC No	CAS No	Classification		Labelling			Spec. Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram, Signal Word Code(s)	Hazard statement code(s)	Suppl. Hazard statement code(s)		
050-027-00-7	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannate-tradecanoate	239-622-4	15571-58-1	Repr. 1B	H360D	GHS08 Dgr	H360D	--	--	--

3. Environmental fate properties

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4. Human health hazard assessment

See information given in Chapter 2 (Harmonised classification and labelling).

4.1. Toxicokinetics (absorption, metabolism, distribution and elimination)

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

² Commission Regulation (EU) No 944/2013 of 2 October 2013 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures

³ Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006

4.2. Acute toxicity

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.3. Irritation

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.4. Corrosivity

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.5. Sensitisation

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.6. Repeated dose toxicity

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.7. Mutagenicity

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.8. Carcinogenicity

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.9. Toxicity for reproduction

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

4.10. Other effects

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

5. Environmental hazard assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

6. Conclusions on the SVHC Properties

6.1. CMR assessment

Pursuant to Annex III of Commission Regulation (EU) No 944/2013 of 2 October 2013 DOTE will be listed in Table 3.1 (List of harmonised classification and labelling of hazardous substances) of Annex VI, part 3, of Regulation (EC) No 1272/2008 as toxic for reproduction Repr. 1B, H360D (May damage the unborn child).

Therefore, this classification of DOTE in Commission Regulation (EC) No 944/2013 shows that the substance meets the criteria for classification as toxic for reproduction in accordance with Article 57 (c) of REACH.

6.2. PBT and vPvB assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

6.3. Equivalent level of concern assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (c).

Annex I - Additional information on human health

DOTe is self-classified by 118 notifiers⁴ indicated in the C&L inventory. In addition to the reproductive toxicity, further hazard endpoints are addressed. A summary is given in Table 3.

Table 3: Self-classification of DOTE in addition to its adverse developmental effects

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Acute Tox. 4	H302 (Harmful if swallowed)
Skin Irrit. 2	H315 (Causes skin irritation)
Skin Sens. 1	H317 (May cause an allergic skin reaction)
STOT RE 1	H372 (Causes damage to thymus through prolonged or repeated exposure via the oral route)
STOT RE 2	H373 (May cause damage to organs through prolonged or repeated exposure)
Aquatic Acute 1	H400 (Very toxic to aquatic life.)
Aquatic Chronic 1	H410 (Very toxic to aquatic life with long lasting effects)

DOTe is (according to the information of registrants) manufactured and marketed as a multi-constituent substance, consisting of DOTE and of the corresponding mono-octyl substance MOTE. Based on the currently available data it can be assumed that the mono-octyl tin compound MOTE has no adverse effect on the reproductive system (MAK, 2012, Arkema, 2009). No harmonised classification exists for MOTE. The self-classification as indicated in the C&L inventory is shown in Table 14.

Table 4: Self-classification of MOTE

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Repr. 2*	H361 (Suspected of damaging the fertility or the unborn child)
Skin Irrit. 2	H315 (Causes skin irritation)
Skin Sens. 1B	H317 (May cause an allergic skin reaction)
STOT RE 1	H372 (Causes damage to thymus through prolonged or repeated exposure via the oral route)
STOT RE 2	H373 (May cause damage to organs through prolonged or repeated exposure)
Aquatic Acute 1	H400 (Very toxic to aquatic life)
Aquatic Chronic 1	H410 (Very toxic to aquatic life with long lasting effects)

*it is assumed that the classification for reproductive toxicity is based on the impurity DOTE and the use of MOTE as multi-constituent substance MOTE:DOTe.

⁴ C&L Inventory database, <http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database> (accessed 02 January 2014)

Reproductive toxicity

The dioctyltin compound DOTE has been identified as Repr. 1B substance based on criteria laid down in Regulation (EC) No 1272/2008. A CLH dossier has been submitted by industry suggesting to classify DOTE as Repr. 2 (H361d: suspected of damaging the unborn child) (CLH Report, 2011). The Committee for Risk Assessment (RAC) decided on the basis of available data that DOTE should be classified as Repr. 1B (RAC, 2012). According to RAC the observed developmental toxicity effects are not considered to be secondary non-specific consequences of the thymus toxicity but are due to adverse effects on the developmental toxicity parameters. The studies showed clear evidence of developmental toxicity in three different species, and there is no information available that these might not be relevant for humans.

Available data indicate that MOT compounds do not have adverse effects on the reproductive system, thus the adverse effects of the reaction mass DOTE:MOTE is related to the presence of DOTE (MAK, 2012).

In a recently conducted developmental screening assay, in which pure MOTE (97.9%) was applied in concentrations up to 1250 mg/kg bw/day orally to Wistar rats, no adverse effects on fertility or on the development were observed (Arkema, 2009), confirming the previous conclusion. A testing proposal for a reproductive toxicity (pre-natal developmental toxicity) study according to OECD test guideline 414 with MOTE has been submitted by the registrant(s).

References

Arkema (2009). Reproduction/developmental toxicity screening assay in rats. TNP Report V7661, Arkema, Frankreich.

CLH Report (2011). Proposal for harmonised classification and labelling based on the regulation (EC) No 1272/2008 (CLP Regulation) Annex VI, Part 2. Substance name: Dioctyltin bis(2-ethylhexyl mercaptoacetate). Dossier Submitter: Arkema on behalf of ETSINA.

MAK – Maximale Arbeitsplatzkonzentration (2012). Nachtrag 2012 N-Octylverbindungen. pp. 6

RAC - Committee for Risk Assessment (2012). Opinion proposing harmonised classification and labelling at EU level of Dioctyltin bis (2-Ethylhexyl mercaptoacetate). ECHA/RAC/CLH-O-00000243-78-01/F