

Substance Name:

Reaction mass of 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate and 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (reaction mass of DOTE and MOTE)

EC Number: -

CAS Number: -

MEMBER STATE COMMITTEE

SUPPORT DOCUMENT FOR IDENTIFICATION OF

REACTION MASS OF 2-ETHYLHEXYL 10-ETHYL-4,4-DIOCTYL-7-OXO-8-OXA-3,5-DITHIA-4-STANNATETRADECANOATE AND 2-ETHYLHEXYL 10-ETHYL-4-[[2-[(2-ETHYLHEXYL)OXY]-2-OXOETHYL]THIO]-4-OCTYL-7-OXO-8-OXA-3,5-DITHIA-4-STANNATETRADECANOATE (REACTION MASS OF DOTE AND MOTE)

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 | Dioctyltin |
| 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(s): Reaction mass of 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate and 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (reaction mass of DOTE and MOTE)

EC Number(s): -

CAS number(s): -

- The reaction mass DOTE:MOTE is identified as substances meeting the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to the classification of DOTE 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, which is together with MOTE the main constituent of the reaction mass, 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 reaction mass DOTE:MOTE 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

The registrants have made use of the option allowing the registration of individual constituents for multi-constituent (reaction mass) substances.²

² ECHA Guidance for identification and naming of substances under REACH and CLP (http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf)

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: | - |
| CAS name: | - |
| IUPAC name: | Reaction mass of 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate and 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-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 (covering DOTE) |
| Molecular formula: | C ₃₆ H ₇₂ O ₄ S ₂ Sn (DOTE) C ₃₈ H ₇₄ O ₆ S ₃ Sn (MOTE) |
| Molecular weight range: | 751.79 (DOTE) 841.90 (MOTE) |
| Synonyms: | <p>Synonyms: DOTE, DOT(EHMA)₂, Di-octyltin 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)dacetate, 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-ethylhexyl)mercaptoacetate)</p> <p>Synonyms: MOTE, MO(EHMA)₃, Mono-octyltin tris(2-ethylhexyl mercaptoacetate), Octyltin tris(2-ethylhexyl mercaptoacetate), Acetic acid, ((octylstannylidyne)trithio)tri-, tris(2-ethylhexyl) ester, Acetic acid, ((octylstannylidyne)trithio)tris-,tris(2-ethylhexyl) ester, Mono-n-octyl-tin-tris-(2-ethylhexyl)mercaptoacetate), Octyltintris(2-ethylhexyl mercaptoacetate), Octyltris(2-ethylhexyloxycarbonylmethylthio)stannane, Tin, octyl-, tris(isooctylthio glycollate), Acetic acid, ((octylstannylidyne)trithio)tris-,tris(2-ethylhexyl) ester</p> |

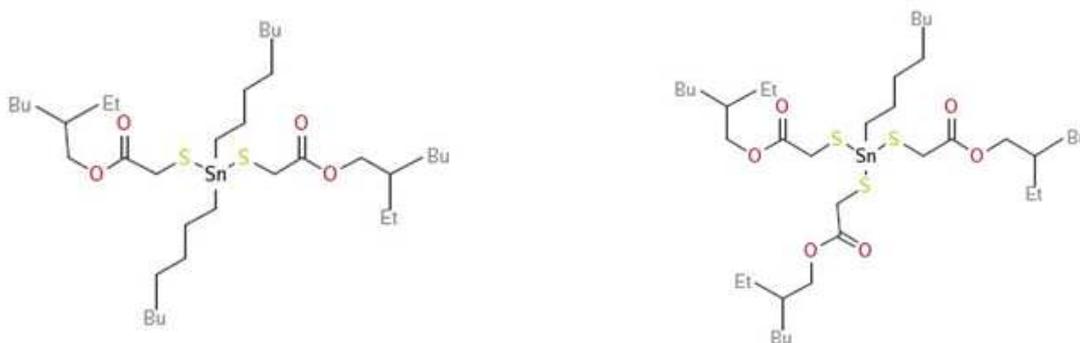
Structural formula:

Figure 1: Structural formula of DOTE (left) and MOTE (right)

It is noted that MOTE and DOTE contain chiral carbon atoms in the ethylhexyl residue of the acetic ester group. The indicated CAS numbers do not reflect any specific stereoisomeric forms. No specification on the stereoisomers of the reaction mass is provided in the registrations. In view of the technical synthesis of MOTE and DOTE and following discussions with experts from the tin-organic stabiliser industry it is assumed, that the reaction mass consists of a racemic mixture of the R- and S- forms. The SVHC dossier covers the substance including all possible stereoisomers.

1.2. Composition of the substance

Name: Reaction mass of 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate and 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate

Description: Multi-constituent substance

Degree of purity: see confidential Annex II (not attached here)

The concentration ratio between DOTE and MOTE in the reaction mass can differ depending on the manufacture of the mixture and depending on the technical needs. All reaction masses with concentrations of DOTE equal or above 10% are covered by this dossier following the definition of a multi-constituent substance (see Table 2).³

Table 2: Composition of the reaction mass DOTE:MOTE

| Constituents | Typical concentration | Concentration Range | Remarks |
|---|---------------------------|---------------------|---|
| 2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (DOTE) EC # 239-622-4 CAS # 15571-58-1 | ≥10% (w/w) and <80% (w/w) | | Overall typical concentration for DOTE. All possible stereoisomers are considered to be the main constituents |
| 2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate (MOTE) EC # 248-227-6 CAS # 27107-89-7 | ≥10% (w/w) and <80% (w/w) | | Overall typical concentration for MOTE. All possible stereoisomers are considered to be the main constituents |

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 MOTE as individual substances². 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, in addition to the present document an Annex XV SVHC dossier was submitted for DOTE for its identification as SVHC.

³ ECHA Guidance for identification and naming of substances under REACH and CLP (http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf)

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 944/2013⁴ as of 2 October 2013 DOTE, which is together with MOTE the main constituent of the reaction mass, 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 1272/2008⁵ as toxic for reproduction Repr. 1B, H360D (May damage the unborn child).

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

The harmonised classification as indicated in Table 3 applies from 1 January 2015.

Table 3: Harmonised classification of DOTE 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 | -- | -- | -- |

MOTE, the corresponding monoctyl compound of DOTE, does not have an entry in Annex VI of Regulation (EC) No 1272/2008.

⁴ 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

⁵ 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

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).

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

Brief information is provided in Annex I.

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 as of 2 October 2013 DOTE, which is together with MOTE the main constituent of the reaction mass, 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 reaction mass DOTE:MOTE meets the criteria for the 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 notifiers⁶ indicated in the C&L inventory. In addition to the harmonised classification further hazard endpoints are addressed. A summary is given in Table 4.

Table 4: 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) |

Based on the currently available data it can be assumed that the mono-octyltin 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 15.

Table 5: 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.

Reproductive toxicity

⁶C&L Inventory database, <http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database> (accessed 02 January 2014)

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-000000243-78-01/F