9 December 2011

**Substance name: Lead 2,4,6 – trinitro-m-phenylene dioxide (lead styphnate)**
**EC number: 239-290-0**
**CAS number: 15245-44-0**

# SUPPORT DOCUMENT FOR IDENTIFICATION OF LEAD STYPHNATE AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR PROPERTIES

# NOTE

During the public consultation, in accordance with Article 59 (4) of the REACH Regulation, on the proposed identification of lead styphnate as a Substance of Very High Concern (SVHC) on the basis of its classification as toxic to reproduction category 1A no comments were received objecting the conclusion that the substance meets criteria set out in Article 57(c). Therefore, in accordance with Article 59 (6), lead styphnate has been included in the Candidate List by ECHA.

The present support document comprises Part I (Justification) of the Annex XV dossier for identification of lead styphnate as SVHC on the basis of Article 57(c) of REACH.

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| **Substance Name:** | **Lead 2,4,6-trinitro-m-phenylene dioxide (lead styphnate)** |
| **EC Number:** | **239-290-0** |
| **CAS Number:** | **15245-44-0** |

- The substance is identified as substance meeting the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to its classification as toxic to reproduction category 1A[1] which corresponds to classification as toxic to reproduction category 1[2].

**Summary of how the substance(s) meet(s) the CMR (1A or 1B) criteria**

Lead styphnate is covered by index numbers 609-019-00-4 and 609-019-01-1 of Regulation (EC) No 1272/2008 and classified in Annex VI, Part 3, Table 3.1 (list of harmonised classification and labelling of hazardous substances) as toxic to reproduction, Repro. 1A ((H360-Df: 'May damage the unborn child. Suspected of damaging fertility'). The corresponding classification in Annex VI, part 3, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is toxic to reproduction category 1 (R61: "May damage the unborn child. Suspected of damaging fertility').

Therefore, this classification of lead styphnate in Regulation (EC) No 1272/2008 shows that the substance meets the criteria for classification as toxic to reproduction in accordance with Article 57 (c) of REACH.

**Registration dossiers submitted for the substance?** Yes

[1] Classification in accordance with Regulation (EC) No 1272/2008 Annex VI, part 3, Table 3.1 List of harmonised classification and labelling of hazardous substances.

[2] Classification in accordance with Regulation (EC) No 1272/2008, Annex VI, part 3, Table 3.2 List of harmonised classification and labelling of hazardous substances (from Annex I to Council Directive 67/548/EEC).

# JUSTIFICATION

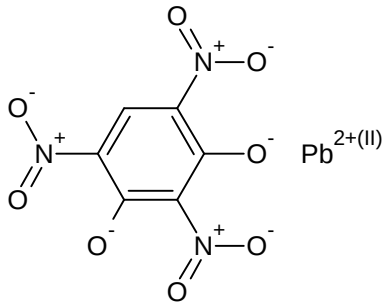
## 1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

### 1.1 Name and other identifiers of the substance

**Table 1.1: Substance identity**

| | |
|---|---|
| **EC number:** | 239-290-0 |
| **EC name:** | lead 2,4,6-trinitro-m-phenylene dioxide |
| **CAS number (in the EC inventory):** | 15245-44-0 |
| **CAS number:** | 15245-44-0<br>66778-13-0 (mono hydrate) |
| **Deleted CAS numbers:** | 4219-19-6; 6594-85-0; 59286-40-7; 63918-97-8 |
| **CAS name:** | 1,3-Benzenediol, 2,4,6-trinitro-, lead(2+) salt (1:1) |
| **IUPAC name:** | Lead(2+) 2,4,6-trinitrobenzene-1,3-diolate |
| **Index number in Annex VI of the CLP Regulation** | 609-019-00-4 |
| **Molecular formula:** | $C_6$ H $N_3$ $O_8$ Pb |
| **Molecular weight:** | 450.3 g/mol |
| **Synonyms:** | 2,4-Dioxa-3-plumbabicyclo[3.3.1]nona-1(9),5,7-triene, 3,3didehydro-6,8,9-trinitro-<br>Lead, [styphnato(2-)]-<br>Resorcinol, 2,4,6-trinitro-, lead(2+) salt (1:1)<br>Lead styphnate<br>Lead tricinate<br>Lead trinitroresorcinate<br>Tricinat |

**Structural formula:**




## 1.2 Composition of the substance

**Name:** lead 2,4,6-trinitro-m-phenylene dioxide

**Description:** not relevant

**Degree of purity:** > 75 – 100%

**Table 1.2: Constituents**

| Constituents | Typical concentration | Concentration range | Remarks |
|---|---|---|---|
| lead 2,4,6-trinitro-m-phenylene dioxide<br>EC number: 239-290-0 | > 90 % | > 75 – 100 % | Based on the registration dossiers received |

**Table 1.3: Impurities**

| Impurities | Typical concentration | Concentration range | Remarks |
|---|---|---|---|
| Confidential information | | > 0 – 21 % | Based on the registration dossiers received |

**Table 1.4: Additives**

| Additives | Typical concentration | Concentration range | Remarks |
|---|---|---|---|
| Confidential information | | | |

## 1.3 Physico-chemical properties

**Table 1.5: Overview of physicochemical properties[3]**

| Property | Value | Remarks | |
|---|---|---|---|
| Physical state at 20°C and 101.3 kPa | Solid<br>Orange or reddish brown rhombical explosive crystals | *Discussion and the value used for Chemical Safety Assessment (CSA) reported in the endpoint summary* | Bornscheuer, U.; Roempp; Georg Thieme Verlag KG, 2008 |
| Melting/freezing point | Decomposing at 190 °C | *idem* | Bornscheuer, U.; Roempp; Georg Thieme Verlag KG, 2008 |
| Water solubility | 0.5 – 0.7 g/l at 20 °C | *idem* | Lawrentz U.; Water solubility based on an „OECD Guideline for the Testing of Chemicals"; RUAG Laboratories, 2010 |
| Partition coefficient n-octanol/water (log value) | -2.19 at 20 °C | *idem* | Determination of the partition coefficient of n-octanol/water of "Lead styphnate" according to OECD 107; RUAG laboratories, 2010 |

[3] *The references of the values reported in Table 5 will be available in the technical dossier. In case references need to be included an additional column could be added manually to Table 5.*

# 2 HARMONISED CLASSIFICATION AND LABELLING

Lead styphnate is covered by Index number numbers 609-019-00-4 and 609-019-01-1 in Annex VI, part 3 of Regulation (EC) No 1272/2008 as follows:

**Table 2.1: Classification according to part 3 of Annex VI, Table 3.1 ((list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008**

| 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) | | |
| 609-019-00-4 | Lead 2,4,6-trinitro-*m*-phenylene dioxide; lead 2,4,6-trinitroresorcinoxide; lead styphnate | 239-290-0 | 15245-44-0 | Unst. Expl.<br>Repr. 1A<br>Acute Tox. 4*<br>Acute Tox. 4*<br>STOT RE 2*<br>Aquatic Acute 1<br>Aquatic Chronic 1 | H200<br>H360-Df<br>H332<br>H302<br>H373**<br>H400<br>H410 | GHS01<br>GHS08<br>GHS07<br>GHS09<br>Dgr | H200<br>H360Df<br>H332<br>H302<br>H373**<br>H410 | | | 1 |
| 609-019-01-1 | Lead 2,4,6-trinitro-*m*-phenylene dioxide; lead 2,4,6-trinitroresorcinoxide; lead styphnate (≥20% phlegmatiser) | 239-290-0 | 15245-44-0 | Expl. 1.1<br>Repr. 1A<br>Acute Tox. 4*<br>Acute Tox. 4*<br>STOT RE 2*<br>Aquatic Acute 1<br>Aquatic Chronic 1 | H201<br>H360-Df<br>H332<br>H302<br>H373**<br>H400<br>H410 | GHS01<br>GHS08<br>GHS07<br>GHS09<br>Dgr | H200<br>H360Df<br>H332<br>H302<br>H373**<br>H410 | | | 1 |

***Note 1:***
*The concentration stated or, in the absence of such concentrations, the generic concentrations of this Regulation (Table 3.1) or the generic concentrations of Directive 1999/45/EC (Table 3.2), are the percentages by weight of the metallic element calculated with reference to the total weight of the mixture.*

**Table 2.2: Classification according to part 3 of Annex VI, Table 3.2 (list of harmonized classification and labelling of hazardous substances from Annex I of Council Directive 67/548/EEC) of Regulation (EC) No 1272/2008**

| Index No | International Chemical Identification | EC No | CAS No | Classification | Labelling | Concentration limits | Notes |
|---|---|---|---|---|---|---|---|
| 609-019-00-4 | Lead 2,4,6-trinitro-*m*-phenylene dioxide; lead 2,4,6-trinitroresorcinoxide; lead styphnate | 239-290-0 | 15245-44-0 | E; R3<br>Repr. Cat. 1;R61<br>Repr. Cat.3; R62<br>Xn; R20/22<br>R33<br>N; R50-53 | E; T; N<br>R: 61-3-20/22-33-50/53-62<br>S: 53-45-60-61 | | E<br>1 |

***Note E (Table 3.2 ) :***
*Substances with specific effects on human health (see Chapter 4 of Annex VI to Directive 67/548/EEC) that are classified as carcinogenic, mutagenic and/or toxic for reproduction in categories 1 or 2 are ascribed Note E if they are also classified as very toxic (T+), toxic (T) or harmful (Xn). For these substances, the risk phrases R20,*

*R21, R22, R23, R24, R25, R26, R27, R28, R39, R68 (harmful), R48 and R65 and all combinations of these risk phrases shall be preceded by the word 'Also'.*

# 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

*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 PBT, vPvB assessment

Not relevant.

## 6.2 CMR assessment

Lead styphnate is covered by index numbers 609-019-00-4 and 609-019-01-1 of Regulation (EC) No 1272/2008 and classified in Annex VI, Part 3, Table 3.1 (list of harmonised classification and labelling of hazardous substances) as toxic to reproduction, Repro. 1A ((H360-Df: 'May damage the unborn child. Suspected of damaging fertility'). The corresponding classification in Annex VI, part 3, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is toxic to reproduction category 1 (R61: "May damage the unborn child. Suspected of damaging fertility').

Therefore, this classification of lead styphnate in Regulation (EC) No 1272/2008 shows that the substance meets the criteria for classification as toxic to reproduction in accordance with Article 57 (c) of REACH.

## 6.3 Substances of equivalent level of concern assessment.

Not relevant.