

## **Annex XV report**

# **PROPOSAL FOR IDENTIFICATION OF SUBSTANCES OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57**

**Substance name:** 2-(4-tert-butylbenzyl)propionaldehyde and its individual stereoisomers

**EC numbers:** -

**CAS numbers:** -

**Submitted by:** Sweden

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## PROPOSAL FOR IDENTIFICATION OF SUBSTANCES OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57

**Substance name:** 2-(4-tert-butylbenzyl)propionaldehyde and its individual stereoisomers

**EC numbers:** -

**CAS numbers:** -

- The substances are proposed to be identified as substances meeting the criteria of Article 57 (c) of Regulation (EC) No 1907/2006 (REACH) owing to the classification of 2-(4-tert-butylbenzyl)propionaldehyde in the hazard class toxic to reproduction category 1B<sup>1</sup>.

### Summary of how the substances meet the criteria set out in Article 57 of the REACH Regulation

2-(4-tert-butylbenzyl)propionaldehyde is covered by index number 605-041-00-3 of Regulation (EC) No 1272/2008 in Annex VI, part 3, Table 3 (the list of harmonised classification and labelling of hazardous substances) and it is classified in the hazard class toxic for reproduction category 1B (H360Fd<sup>2</sup>).

Therefore, this classification of the substance in Regulation (EC) No 1272/2008 shows that the substances meet the criteria for classification in the hazard class:

- toxic for reproduction category 1B in accordance with Article 57 (c) of REACH.

### Registration dossiers submitted for the substance:

- Yes (2-(4-tert-butylbenzyl)propionaldehyde)
- No ((2S)-3-(4-tert-butylphenyl)-2-methylpropanal, (2R)-3-(4-tert-butylphenyl)-2-methylpropanal)

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<sup>1</sup> Classification in accordance with section 3.7 of Annex I to Regulation (EC) No 1272/2008.

<sup>2</sup> H360Fd: "May damage fertility. Suspected of damaging the unborn child".

## PART I

### Justification

#### 1. Identity of the substance and physical and chemical properties

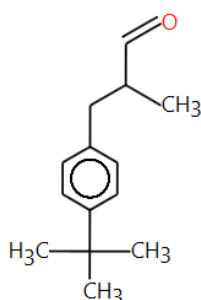
In the manufacturing process of 2-(4-tert-butylbenzyl)propionaldehyde the substance is obtained as racemic mixture (1:1) of the two enantiomers (2S)-3-(4-tert-butylphenyl)-2-methyl-propanal (CAS 75166-30-2) and (2R)-3-(4-tert-butylphenyl)-2-methyl-propanal (CAS 75166-31-3)<sup>3</sup>.

##### 1.1 Name and other identifiers of the substances

**Table 1: Substance identity 2-(4-tert-butylbenzyl)propionaldehyde**

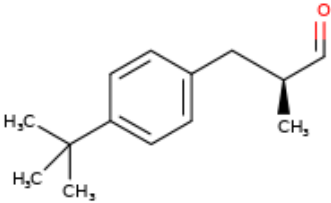
<b>EC number:</b>	201-289-8
<b>EC name:</b>	2-(4-tert-butylbenzyl)propionaldehyde
<b>CAS number (in the EC inventory):</b>	80-54-6
<b>Deleted CAS numbers:</b>	39390-70-0 75166-25-5
<b>CAS name:</b>	Benzenepropanal, 4-(1,1-dimethylethyl)- $\alpha$ -methyl-
<b>IUPAC name:</b>	3-(4- <i>tert</i> -butylphenyl)-2-methylpropanal
<b>Index number in Annex VI of the CLP Regulation</b>	605-041-00-3
<b>Molecular formula:</b>	C <sub>14</sub> H <sub>20</sub> O
<b>Molecular weight range:</b>	204.308
<b>Synonyms:</b>	Lilial Lilestralis 2-Methyl-3-(4-tert-butylphenyl)propanal

##### Structural formula:

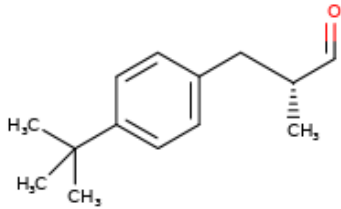


<sup>3</sup> CLH report for 2-(4-tert-butylbenzyl)propionaldehyde, 2017.

**Table 2: Substance identity (2S)-3-(4-tert-butylphenyl)-2-methylpropanal**

<b>EC number:</b>	-
<b>EC name:</b>	-
<b>CAS number (in the EC inventory):</b>	75166-30-2
<b>Deleted CAS numbers:</b>	
<b>CAS name:</b>	Benzenepropanal, 4-(1,1-dimethylethyl)- $\alpha$ -methyl-, ( $\alpha$ S)-
<b>IUPAC name:</b>	(2S)-3-(4- <i>tert</i> -butylphenyl)-2-methylpropanal
<b>Index number in Annex VI of the CLP Regulation</b>	
<b>Molecular formula:</b>	C <sub>14</sub> H <sub>20</sub> O
<b>Molecular weight range:</b>	204.308
<b>Structural formula:</b>	

**Table 3: Substance identity (2R)-3-(4-tert-butylphenyl)-2-methylpropanal**

<b>EC number:</b>	-
<b>EC name:</b>	-
<b>CAS number (in the EC inventory):</b>	75166-31-3
<b>Deleted CAS numbers:</b>	
<b>CAS name:</b>	Benzenepropanal, 4-(1,1-dimethylethyl)- $\alpha$ -methyl-, ( $\alpha R$ )-
<b>IUPAC name:</b>	(2R)-3-(4-tert-butylphenyl)-2-methylpropanal
<b>Index number in Annex VI of the CLP Regulation</b>	
<b>Molecular formula:</b>	C <sub>14</sub> H <sub>20</sub> O
<b>Molecular weight range:</b>	204.308
<b>Structural formula:</b>	

## 1.2 Composition of the substance

The dossier applies to both the racemate and its individual enantiomers.

**Name:** 2-(4-tert-butylbenzyl)propionaldehyde and its individual stereoisomers

**Description:** organic

**Substance type:** -

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

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

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

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

## 1.5 Physicochemical properties

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

## 2. Harmonised classification and labelling

2-(4-tert-butylbenzyl)propionaldehyde is covered by Index number 605-041-00-3 in part 3 of Annex VI to the CLP Regulation as follows:

**Table 4: Classification according to Annex VI, Table 3 (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)		
605-041-00-3	2-(4-tert-butylbenzyl)propionaldehyde	201-289-8	80-54-6	Repr. 1B	H360Fd	GHS08 Dgr	H360Fd			

## 3. Environmental fate properties

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

## 4. Human health hazard assessment

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

## 5. Environmental hazard assessment

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



## **6. Conclusions on the SVHC Properties**

### **6.1 CMR assessment**

2-(4-tert-butylbenzyl)propionaldehyde is covered by index number 605-041-00-3 of Regulation (EC) No 1272/2008 in Annex VI, part 3, Table 3 (the list of harmonised classification and labelling of hazardous substances) and it is classified in the hazard class toxic for reproduction category 1B (H360Fd<sup>4</sup>).

Therefore, this classification of the substance in Regulation (EC) No 1272/2008 shows that the substances meet the criteria for classification in the hazard class:

- toxic for reproduction category 1B in accordance with Article 57 (c) of REACH.

### **6.2 PBT and vPvB assessment**

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

### **6.3 Assessment under Article 57(f)**

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

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<sup>4</sup> H360Fd: "May damage fertility. Suspected of damaging the unborn child".

## Part II

### 7. Registration and C&L notification status

#### 7.1 Registration status

**Table 5: Registration status**

From the ECHA dissemination site <sup>5</sup>	
Registrations	<input checked="" type="checkbox"/> Full registration(s) (Art. 10)  <input type="checkbox"/> Intermediate registration(s) (Art. 17 and/or 18)

#### 7.2 CLP notification status

**Table 6: CLP notifications**

	CLP Notifications <sup>6</sup>
Number of aggregated notifications	51
Total number of notifiers	2252

### 8. Total tonnage of the substance

**Table 7: Tonnage status**

Total tonnage band for the registered substance (excluding the volume registered under Art 17 or Art 18) <sup>7</sup>	1000 - 10 000 t/pa
Tonnage information from public sources other than registration dossiers (if available)	No information

<sup>5</sup> <https://echa.europa.eu/sv/registration-dossier/-/registered-dossier/13572> (accessed 01-09-2020)

<sup>6</sup> C&L Inventory database, <http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database> (accessed 29-12-2020)

<sup>7</sup> <https://echa.europa.eu/sv/registration-dossier/-/registered-dossier/13572> (accessed 01-09-2020)

## 9. Information on uses of the substance

Table 8: Uses

	Uses	Registered use	Use possibly in the scope of Authorisation
<b>Uses as intermediate</b>			
<b>Formulation or repacking</b>	<p><u>Compounding</u></p> <p>ERC: 2 (Formulation into mixture)</p> <p>PROC: 1, 2, 3 (Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions), 5 (Mixing or blending in batch processes), 8a (Transfer of substance or mixture (charging and discharging) at non-dedicated facilities), 8b, 9, 15</p> <p><u>Formulation</u></p> <p>ERC: 2</p> <p>PROC: 1, 2, 3, 4 (Chemical production where opportunity for exposure arises), 5, 8a, 8b, 9, 14 (Tabletting, compression, extrusion, pelletisation, granulation), 15</p>	Yes	Yes
<b>Uses at industrial sites</b>	<p><u>Use at industrial site as a chemical intermediate</u></p> <p>ERC: 6a (Use of intermediate)</p> <p>PROC: 1, 2, 8b</p> <p>SU: 8 (Manufacture of bulk, large scale chemicals including petroleum products)</p> <p><u>Use in Cleaning agents</u></p> <p>ERC: 4 (Use of non-reactive processing aid at industrial site (no inclusion into or onto article))</p> <p>PROC: 1, 2, 4, 5, 7 - Use in Cleaning agents - industrial Chain maintenance/foam/ animal housing/ disinfection fogging gassing - food/pharma, 8a, 8b 10 (Roller application or brushing), 13 (Treatment of articles by dipping and pouring)</p> <p>PC: 35 (Washing and cleaning products)</p>	Yes	No  Yes
<b>Uses by professional</b>	<u>Use in Cleaning Agents</u>	Yes	Yes

ANNEX XV – IDENTIFICATION OF 2-(4-TERT-BUTYLBENZYL)PROPIONALDEHYDE AND ITS INDIVIDUAL STEREOISOMERS AS SVHC

<p><b>workers</b></p>	<p>ERC: 8a (Widespread use of non-reactive processing aid (no inclusion into or onto article, indoor)), 8d (Widespread use of non-reactive processing aid (no inclusion into or onto article, outdoor))</p> <p>PROC: 1, 2, 4, 8a, 8b, 11 (Non-industrial spraying), 13, 19 (Hand-mixing with intimate contact and only PPE available)</p> <p>PC: 31 (Polishes and wax blends), 35</p> <p>SU: 10 (Formulation [mixing] of preparations and/or re-packaging (excluding alloys))</p>		
<p><b>Consumer uses</b></p>	<p><u>Use in Air Care</u></p> <p>ERC: 8a</p> <p>PC: 3 (Air care products)</p> <p><u>Use in Cleaning Agents</u></p> <p>ERC: 8a, 8d</p> <p>PC: 31, 35</p> <p><u>Consumer end-use of biocidal products</u></p> <p>ERC: 8a, 8d</p> <p>PC: 8 (Biocidal products, e.g. disinfectants, pest control),</p> <p><u>Professional and consumer end-use of cosmetics</u></p> <p>ERC: 8a</p> <p>PC: 28 (Perfumes, fragrances), 39 (Cosmetics, personal care products)</p> <p><u>Other consumer Use: Coatings and paints, thinners, paint removes; Fillers, putties, plasters, modelling clay; Finger paints, Ink and toners</u></p> <p>ERC: 8a, 8d</p> <p>PC: 8 9a (Coatings and paints, thinners, paint removes), 9b (Fillers, putties, plasters, modelling clay), 9c (Finger paints), 18 (Ink and toners)</p> <p><u>Industrial, Professional and Consumer end-use of washing and cleaning products</u></p> <p>ERC: 8a</p> <p>PC: 35</p> <p><u>Consumer and Professional end-use of</u></p>	<p>Yes</p>	<p>Yes</p>

	<p><u>polishes and wax blends</u></p> <p>ERC: 8a</p> <p>PC: 31</p>		
<b>Article service life</b>	<p><u>Use of substances in scented articles</u></p> <p>AC: 0 (Other: Scented articles)</p> <p>ERC: 11a (Widespread use of articles with low release (indoor))</p>	Yes	Yes

## 10. Information on structure of the supply chain

No information available.

## 11. Additional information

### 11.1 Alternatives

The substance 3-(4-isobutyl-2-methylphenyl)propanal has been proposed as a possible alternative to 2-(4-tert-butylbenzyl)propionaldehyde (Laue et al. 2017).

### 11.2 Existing EU legislation

2-(4-tert-butylbenzyl)propionaldehyde is included in Annex III of the Cosmetic Products Regulation and is therefore a restricted substance. The presence of the substance must be indicated in the list of ingredients referred to in Article 19(1)(g) when its concentration exceeds: 0.001% in leave-on products and 0.01 % in rinse-off products (Annex III of Regulation (EC) no 1223/2009).

2-(4-tert-butylbenzyl)propionaldehyde is included in Annex II of the Toy Safety Directive and toys containing this substance at concentrations of 100 mg/kg or higher must be labelled accordingly (Annex II of Directive 2009/48/EC).

### 11.3 Previous assessments by other authorities

An opinion on 2-(4-tert-butylbenzyl)propionaldehyde from the Scientific Committee for Consumer Safety (SCCS) acknowledges that male reproductive toxicity has been consistently observed in several different studies. The SCCS states that “*On individual product basis, Butylphenyl methylpropional (p-BMHCA) (CAS 80-54-6) with alpha-tocopherol at 200 ppm, can be considered safe when used as fragrance ingredient in different cosmetic leave-on and rinse-off type products. However, considering the first-tier deterministic aggregate exposure, arising from the use of different product types together, Butylphenyl methylpropional at the proposed concentrations cannot be considered as safe*”. The SCCS mentions that evaluations under REACH or other scientific bodies should be considered in future assessments of 2-(4-tert-butylbenzyl)propionaldehyde as a cosmetic ingredient (SCCS 2019).

## REFERENCES

### References for Part I

EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC. Official Journal of the European Union, L396: 1-849.

EU (2008). Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packing of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006. Official Journal of the European Union, L353: 1-1355.

### References for Part II

EU (2009). Regulation (EC) No 1223/2009 of the European Parliament and of the Council of 30 November 2009 on cosmetic products. Official Journal of the European Union, L342: 59-209.

EU (2009). Directive 2009/48/EC of the European Parliament and of the Council of 18 June 2009 on the safety of toys. Official Journal of the European Union, L170: 1-37.

Laue, H., Kern, S., Badertscher, R. P., Ellis, G., Natsch, A. (2017): p-Alkyl-Benzoyl-CoA Conjugates as Relevant Metabolites of Aromatic Aldehydes With Rat Testicular Toxicity-Studies Leading to the Design of a Safer New Fragrance Chemical. *Toxicol Sci*, 160(2), 244–255.

Scientific Committee on Consumer Safety (2019): Opinion on the safety of Butylphenyl methylpropional (p-BMHCA) in cosmetic products.