

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

EC Number: -

CAS Number: -

**SUPPORT DOCUMENT FOR IDENTIFICATION OF
2-(4-TERT-BUTYLBENZYL)PROPIONALDEHYDE
AND ITS INDIVIDUAL STEREOISOMERS AS
SUBSTANCES OF VERY HIGH CONCERN BECAUSE
OF THEIR TOXIC FOR REPRODUCTION (ARTICLE
57C) PROPERTIES**

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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 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 1B¹.

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 (H360Fd²).

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)

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

² H360Fd: "May damage fertility. Suspected of damaging the unborn child".

Justification

1. Identity of the substance and physical and chemical properties

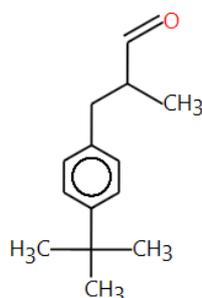
In the manufacturing process of 2-(4-tert-butylbenzyl)propionaldehyde the substance is obtained as racemic mixture (1:1) of the two enantiomers (2S)-3-(4-tert-butylphenyl)-2-methyl-propanal (CAS 75166-30-2) and (2R)-3-(4-tert-butylphenyl)-2-methyl-propanal (CAS 75166-31-3)³.

1.1 Name and other identifiers of the substances

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

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

Structural formula:



³ CLH report for 2-(4-tert-butylbenzyl)propionaldehyde, 2017.

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

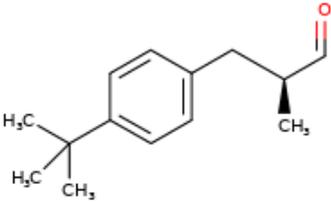
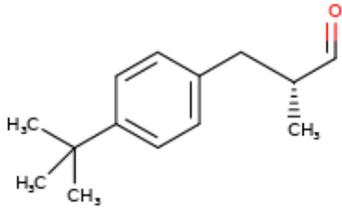
EC number:	-
EC name:	-
CAS number (in the EC inventory):	75166-30-2
Deleted CAS numbers:	
CAS name:	Benzenepropanal, 4-(1,1-dimethylethyl)- α -methyl-, (α S)-
IUPAC name:	(2S)-3-(4- <i>tert</i> -butylphenyl)-2-methylpropanal
Index number in Annex VI of the CLP Regulation	
Molecular formula:	C ₁₄ H ₂₀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

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

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

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 (H360Fd⁴).

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.

⁴ H360Fd: "May damage fertility. Suspected of damaging the unborn child".

REFERENCES

- 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.