Committee for Risk Assessment

RAC

Annex 1

Background document

to the Opinion proposing harmonised classification and labelling at Community level of

reaction mass of

2,4,4-trimethylpent-1-ene

and

2,4,4-trimethylpent-2-ene

ECHA/RAC/ CLH-O-0000001744-73-01/A1

EC number: 246-690-9
CAS number: 25167-70-8

Adopted

10 June 2011

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PROPOSAL FOR HARMONISED CLASSIFICATION AND LABELLING

The classification of 2,4,4-trimethylpentene has been agreed of the TC C&L in September 2009. All endpoints have been addressed within this C&L proposal, since 2,4,4-trimethylpentene was a priority substance in the existing chemicals program (EEC) 793/93. The toxicological information present in this report is the same as that considered by the TC C&L in 2007 because no further data or relevant information was submitted for 2,4,4-Trimethylpentene thereafter. With respect to physical-chemical properties the classification for formation of explosive peroxides (SDS: R19; CLP: EUH019) has been further proposed by the dossier submitter (DS) and discussed in RAC but is not a conclusion taken over from the conclusions in TC C&L group.

From the public consultation four Member States Competent Authorities (CA) comments were received. All supported the flammability and human health classification. Three of the CAs furthermore supported the R19 / EUH019 classification, whereas one industry (IND) comment opposed this classification. Following the discussions RAC does not consider that this classification applies to the substance and, therefore, RAC finds the use of Note D applicable.

Substance Name: **reaction mass of 2,4,4-trimethylpent-1-ene and 2,4,4-trimethylpent-2-ene**

EC Number: **246-690-9**

CAS Number: 25167-70-8

Registration number (s):

Purity: minimum ≥ 90 %

Proposed classification based on Regulation (EC) No 1272/2008 criteria:

	Classification	Wording
Hazard classes, Hazard categories	Flam. Liq. 2 Asp. Tox. 1 STOT SE 3	
Hazard statements	H225 H304 H336	Highly flammable liquid and vapour May be fatal if swallowed and enters airways May cause drowsiness or dizziness

(Note: A harmonisation of the classification for the environmental hazards was not proposed in this dossier.)

Proposed classification based on Directive 67/548/EEC criteria:

	Classification	Wording
Hazard Symbols, Indications of danger	F Xn	Highly flammable Harmful
R-phrases	R11 R65 R67	Highly flammable Harmful: may cause lung damage if swallowed Vapours may cause drowsiness and dizziness

(Note: A harmonisation of the classification for the environmental hazards was not proposed in this dossier.)

Proposed labelling based on Regulation (EC) No 1272/2008

	Labelling	Wording
Pictograms	GHS02 GHS07 GHS08	
Signal Word	Danger	
Hazard statements	H225 H304 H336	Highly flammable liquid and vapour May be fatal if swallowed and enters airways May cause drowsiness or dizziness

Proposed labelling based on Directive 67/548/EEC

	Labelling	Wording
Hazard Symbols, Indications of danger	F Xn	Highly flammable Harmful
R-phrases	R11 R65 R67	Highly flammable Harmful: may cause lung damage if swallowed Vapours may cause drowsiness and dizziness
S-phrases	(S2) S46	Keep out of the reach of children If swallowed, seek medical advice immediately and show this container or label

Proposed specific concentration limits (if any): None

Proposed notes (if any): D

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name: Pentene, 2,4,4-trimethyl-

EC Name: 2,4,4-trimethylpentene

CAS Number: 25167-70-8

IUPAC Name: reaction mass of 2,4,4-Trimethylpent-1-ene and 2,4,4-Trimethylpent-2-ene

1.2 Composition of the substance

For each constituent/ impurity/ additive, fill in the following table (which should be repeated in case of more than one constituent). The information is particularly important for the main constituent(s) and for the constituents (or impurity) which influence the outcome of the dossier.

Chemical Name: 2,4,4-trimethylpent-1-ene

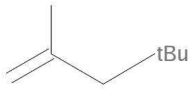
EC Number: 203-486-4

CAS Number: 107-39-1

IUPAC Name: 2,4,4-trimethylpent-1-ene

Molecular Formula: C_8H_{16}

Structural Formula:



Molecular Weight: 112.2 g/mol

Typical concentration (% w/w): Confidential

Concentration range (% w/w): Confidential

Chemical Name: 2,4,4-trimethylpent-2-ene

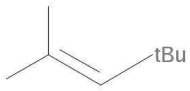
EC Number: 203-488-5

CAS Number: 107-40-4

IUPAC Name: 2,4,4-trimethylpent-2-ene

Molecular Formula: C_8H_{16}

Structural Formula:



Molecular Weight:	112.2 g/mol
Typical concentration (% w/w):	Confidential
Concentration range (% w/w):	Confidential

1.3 Physico-chemical properties

Table 1.1 Summary of physico- chemical properties

REACH ref Annex, §	Property	IUCLID section	Value	[enter comment/reference or delete column]
VII, 7.1	Physical state at 20°C and 101.3 kPa	4.1	colourless liquid at 20 °C, 10.13 kPa	RÖMPP Chemie Lexikon Online (2007)
VII, 7.2	Melting/freezing point	4.2	< -50 °C (freezing point)	Shell Research (1997)
VII, 7.3	Boiling point	4.3	101.4 – 103.6 °C at 1 013 hPa (method according to Siwoloboff)	Shell Research (1997)
VII, 7.4	Relative density	4.4 density	0.7166 at 20 °C (hydrometer method)	Shell Research (1997)
VII, 7.5	Vapour pressure	4.6	57.90 hPa at 25 °C (static method)	Shell Research (1996)
VII, 7.6	Surface tension	4.10	69.9 mN/m at 20 °C c: ca. 1.6 mg/l (ring method)	Shell Research (1997)
VII, 7.7	Water solubility	4.8	1.8 mg/l at 20 °C (flask method)	Shell Research (1997)
VII, 7.8	Partition coefficient n-octanol/water (log value)	4.7 partition coefficient	5.0 at 25 °C (HPLC-method)	Shell Research(1997)
VII, 7.9	Flash point	4.11	-7 °C (closed cup)	Expert judgement by PTB (1996)
VII, 7.10	Flammability	4.13	Pyrophoric properties: The classification procedure need not to be applied because the organic substance is known to be stable into contact with air at room temperature for prolonged periods of time (days). Flammability in contact with water: The classification procedure need not to be applied because the organic substance does not contain metals or metalloids. Explosion limits in air:	BAM II.2 (2010)

			Lower: 0,7 vol% *Upper: 5,8 vol%*	*SDS, Erdölchemie (10/93)*
VII, 7.11	Explosive properties	4.14	The classification procedure need not to be applied because there are no chemical groups present in the molecule which are associated with explosive properties, but 2,4,4-Trimethylpentene may form unstable peroxides by auto-oxidation on contact with air. Due to this classifying with R19 was further proposed by the DS.	BAM II.2 (2010) Reference: P. G. Urben (Ed.): *Bretherick's Handbook of Reactive Chemical Hazards*, 7th ed., Elsevier 2007.
VII, 7.12	Self-ignition temperature	4.12	380 °C *(DIN 51794)*	Expert judgement by PTB (1996)
VII, 7.13	Oxidising properties	4.15	The classification procedure need not to be applied because the organic substance does not contain oxygen, fluorine or chlorine.	*BAM II.2 (2010)*
VII, 7.14	Granulometry	4.5	---	---
XI, 7.15	Stability in organic solvents and identity of relevant degradation products	4.17	---	---
XI, 7.16	Dissociation constant	4.21	---	---
XI, 7.17,	Viscosity	4.22	---	---
	Reactivity towards container material	4.18	---	---
	Thermal stability	4.19	---	---
	Henry's law constant	4.23	$2.127 \cdot 10^5$ Pa· m³· mol^{-1}	Lyman et al. (1982)

2 MANUFACTURE AND USES

2.1 Manufacture

2.2 Identified uses

2.3 Uses advised against

3 CLASSIFICATION AND LABELLING

3.1 Classification in Annex I of Directive 67/548/EEC

NA

3.2 Self classification(s)

4 ENVIRONMENTAL FATE PROPERTIES

Not evaluated for this dossier.

5 HUMAN HEALTH HAZARD ASSESSMENT

5.1 Toxicokinetics (absorption, metabolism, distribution and elimination)

No data are available on 2,4,4-trimethylpentene.

Results from studies on structurally similar compounds:

Nose-only exposure of rats (300 g) to 2,3,4-trimethylpentane which represents a structurally similar but saturated compound resulted in a normalized uptake rate of 4-6 nmol/min per kg bw per ppm (exposure to 100 ppm, flow rate 400 ml/min for 80 min) (Dahl et al., 1988). The uptake rate refers to uptake during minutes 60 to 70 from start of exposure as determined by gas chromatographic measurements of inhaled and exhaled air. From these data it was calculated that approximately 7-

11% of the 2,3,4-trimethylpentane was retained and a value of 10% is proposed to be taken forward for risk characterisation purposes.

There are no studies available on oral or dermal absorption. From the physico-chemical data (log P 5.0, water solubility 1.8 mg/l, molecular weight 112 g/mol) the substance shows a good oral and dermal bioavailability. It is proposed to take forward for the risk characterisation a value of 100%.

In vitro studies on short chain olefins (n-1-octene, n-4-octene, and 3-ethyl-2-pentene) with rat liver microsomes demonstrated the conversion of olefins to diols via epoxide intermediates (Maynert et al., 1970). Similar reactions can be assumed for 2,4,4-trimethylpentene although the quantitative extent remains to be determined.

5.2 Acute toxicity

5.3 Irritation

5.4 Corrosivity

5.5 Sensitisation

5.6 Repeated dose toxicity

5.7 Mutagenicity

5.8 Carcinogenicity

5.9 Toxicity for reproduction

5.10 Other effects

5.10.1 Aspiration toxicity hazard:

In the draft RAR of 2007, the assessment was based on the following argumentation:

The assessment of the aspiration hazard posed by C6-C14 olefins is not based on EU classification criteria but on human experience summarised within a list of data compiled by the Shell Oil Company resulting in the statement: "Aspiration is a significant hazard with C6-C14 olefins". Similar considerations are mentioned in the Martindale Extra Pharmacopoeia published in 1982, stating on page 1452 for light petroleum: "Adverse Effects and Treatment. As for Kerosene, light petroleum and petrol, being more volatile than kerosene, are more likely to the inhaled and to cause aspiration pneumonitis. The toxicity of petrol varies with its composition". Hence, on the basis of

the experience gained by producers of C8 olefins, we suggest that classification with R65 is warranted.

Criteria for classification

Aspiration toxicity hazard category 1 (Asp. Tox. 1) / R65 (Harmful: may cause lung damage if swallowed) / is also warranted for liquid substances and preparations because of their low viscosity. Low viscosity leads to flow and low surface tension leads to spread of a liquid through the respiratory tract.

Aspiration toxicity hazard category 1 (Asp. Tox. 1) is also warranted, if the substance is a hydrocarbon and has a kinematic viscosity *v* of 20.5 mm^2/s or less, measured at 40°C (Regulation (EC) No 1272/2008, section 3.10.2).

R65 is warranted, if the substance is a hydrocarbon and has a kinematic viscosity *v* of less than 7 x 10^{-6} m^2/s (= 7 mm^2/s) at 40ºC (Directive 67/548/EEC).

While there is limited data on the viscosity of 2,4,4-trimethylpentene at different temperatures, the dynamic viscosity η of liquid organic compounds can be approximated on the basis of the De Guzman-Andrade equation (van Velzen et al. 1972):

$$\eta = 10^{B\cdot\left(\frac{1}{T}-\frac{1}{T_0}\right)} \qquad [mPa\cdot s]$$

T is the Temperature, and T_0 and B are two calculable variables (see section 7.1.1 for more details):

Method 1: η = 0.4183 mPa·s

A second method is based on the normal boiling point, the number of carbons and the compound class (Grain 1990). The viscosity at the boiling point Tb is given (0.2 mPa·s), as well as a constant K_F relating to the structure. Another parameter n does not describe number of carbons but rather a tabulated value for the compound class (see section 7.1.2 for more details):

$$\eta = \eta_B \cdot e^{B_4\cdot\left(\frac{1}{T}-\frac{1}{T_b}\right)} \qquad [mPa\cdot s]$$

Method 2: η = 0.0735 mPa·s

The kinematic viscosity *v* relates to the dynamic viscosity via the density *ρ*:

$$\nu = \frac{\eta}{\rho}$$

With density ρ = 0.7166 $g\cdot cm^{-3}$.

From Method 1 with a dynamic viscosity η = 0.4183 mPa·s, the kinematic viscosity of 2,4,4-trimethylpentene at 40°C is approximately 0.58 mm^2/s, which is less than 20.5 mm^2/s / 7 mm^2/s, and requires labelling as proposed (see *Conclusion*).

From Method 2 with a dynamic viscosity η = 0.0727 mPa·s, the kinematic viscosity of 2,4,4-trimethylpentene at 40°C is approximately 0.10 mm^2/s, which supports the other calculated value for kinematic viscosity, and requires labelling as proposed:

Conclusion: 2,4,4-trimethylpentene is a branched hydrocarbon. It is 5 carbons long with 8 carbons in total and has a kinematic viscosity lower than 20.5 mm^2/s / 7 mm^2/s.

Based on human experience as well as physico-chemical properties it is concluded to classify 2,4,4-trimethylpentene as:

Aspiration toxicity category 1 (Asp. Tox. 1) H304 May be fatal if swallowed and enters airways

Xn; R65 Harmful: may cause lung damage if swallowed.

5.10.2 Specific target organ toxicity – single exposure: narcotic effects

Wistar rats (weight 160-210 g) were exposed for four hours (whole body exposure) to six different mist concentrations ranging from 7.6 to 44.0 mg/l. The substance was a mixture of C8 olefins (approx. 75% 2,4,4-trimethylpentene-1 and approx. 15% 2,4,4-trimethlypentene-2). Twenty male and twenty female rats were used in each group/concentration. Mortality was noted starting at concentrations of 21 – 25 mg/l and the LC_{50} was 31.5 mg/l (6 870 ppm) for male rats and 30.0 mg/l (6 540 ppm) for female rats. Exposure (concentration 21.6 mg/l; 4 900 ppm) of ten male and ten female Wistar rats for four hours/day and on five consecutive days resulted in death in 3/10 males and 2/10 females. Animals died within 24 hours. Clinical signs in surviving animals consisted of convulsions, followed by sedation and respiratory distress (Bayer AG, 1972).

Data from structurally analogous substance:

2,2,4-trimethylpentane (CAS No 540-84-1) is classified as R67 (Vapours may cause drowsiness and dizziness). In a five day inhalation study with repeated exposure with 13.2 or 21.6 mg/L and a 14-day observation period, male and female Wistar rats exhibited sedation and impeded breathing among others (Bayer AG 1972).

Criteria for classification based on data from animal studies

Classification for narcotic effects “STOT Single 3” (May cause drowsiness or dizziness) is warranted, if data from animal toxicity studies showing clear symptoms of central nervous system depression (Regulation (EC) No 1272/2008). No concentration limit has been set in the criteria.

R67 (Vapours may cause drowsiness and dizziness) is warranted, if data from animal inhalation toxicity studies showing clear symptoms of central nervous system (CNS) depression at concentrations/exposure times not exceeding 20 mg/l/4h (Directive 67/548/EEC).

Conclusion: Results from the available animal study have shown that 2,4,4-trimethylpentene causes clear signs of CNS depression which requires labelling as STOT Single 3 (May cause drowsiness or dizziness).

With respect to Directive 67/548/EEC, R67 (Vapours may cause drowsiness and dizziness) is proposed. Based on the above data from an animal study, clear signs of CNS effects such as convulsions were evident at exposure concentration of 21.6 mg/l. Although little above the concentration limit of (20 mg/l/4h), this concentration is considered to be still in the range of upper limit concentration for classification.

It is proposed to classify 2,4,4-trimethylpentene as

Specific target organ toxicity – single exposure, category 3 (STOT–SE 3) H336 (May cause drowsiness or dizziness)

Xn; R67 (Vapours may cause drowsiness and dizziness).

5.11 Derivation of DNEL(s) or other quantitative or qualitative measure for dose response

Not relevant for this type of dossier.

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

6.1 Explosivity

No experimental data on explosive properties:
Testing can be waived based on a consideration of the chemical structure in accordance with REACH Column 2 of Annex VII, section 7.11:
The classification procedure needs not to be applied because there are no chemical groups present in the molecule which are associated with explosive properties.

No classification for explosivity is proposed.

2,4,4-Trimethylpentene is a peroxidisable chemical because it contains an **allylic hydrogen (C=C-CH-)** and Bretherick[1] gives guidance and examples of specific compounds and structural types for identifying substances which form explosive peroxides. Due to this classifying with R19/EUH019 was proposed by the DS.

RAC does not consider that this classification apply to the substance, as reference to the more general description in *Bretherick's Handbook of Reactive Chemical Hazards* and not specifically addressing trimethylpentene is not considered sufficient evidence. Also no other alkenes have been classified on Annex VI for this end-point. Although peroxide formation may occur the extent of this in order to form risk for explosion has not been described. From IND comments and in a SDS it is stated that decomposition and polymerisation may occur and that commercial trimethylpentene is supplied with an inhibitor (antioxidant).

Therefore RAC finds the use of note D applicable.

> **Note D:**
>
> Certain substances which are susceptible to spontaneous polymerisation or decomposition are generally placed on the market in a stabilised form. It is in this form that they are listed in Part 3.
>
> However, such substances are sometimes placed on the market in a non-stabilised form. In this case, the supplier must state on the label the name of the substance followed by the words "non-stabilised".

6.2 Flammability

2,4,4-trimethylpentene meets the classification criteria as highly flammable liquid: The flash point measured in a closed cup is -7 °C and with a boiling point at 101.4 – 103.6 °C.

[1] P. G. Urben (Ed.): *Bretherick's Handbook of Reactive Chemical Hazards*, 7th ed., Elsevier 2007.

Proposed classification based on Directive 67/548/EEC:
F, R11 Highly flammable

Proposed classification based on Regulation (EC) No 1272/2008:
Flam. Liq. 2; H225 Highly flammable liquid and vapour

6.3 Oxidising potential

No experimental data on oxidising properties:
Testing can be waived based on a consideration of the chemical structure in accordance with REACH Column 2 of Annex VII, section 7.13: The classification procedure need not to be applied because the organic substance does not contain oxygen, fluorine or chlorine.

No classification for oxidising properties is proposed.

7 ENVIRONMENTAL HAZARD ASSESSMENT

Not evaluated for this dossier.

JUSTIFICATION THAT ACTION IS REQUIRED ON A COMMUNITY-WIDE BASIS

2,4,4-trimethylpentene is a TC C&L agreed substance. All endpoints have been addressed within this C&L proposal, since 2,4,4-trimethylpentene was a priority substance in the existing chemicals program (EEC) 793/93. The proposal to classify with Xn; R65 (based on human data) and omit Xi; R37/38 was already submitted to TC C&L and was agreed on in September 2007. F; R11 and R67 (STOT SE 3, H336) were agreed on in follow-up I and II.

The toxicological information present in this report is the same at that considered by the TC C&L in 2007 because no further data or relevant information was submitted for 2,4,4-trimethylpentene thereafter.

OTHER INFORMATION

7.1 Calculation of dynamic viscosity

7.1.1 Method 1 (van Velzen et al. 1972):

Aspiration toxicity hazard category 1 is also warranted, if the substance is a hydrocarbon and has a kinematic viscosity *v* of 20.5 mm^2/s or less, measured at 40°C (EC Regulation No 1272/2008, section 3.10.2). While there is limited data on the viscosity of 2,4,4-trimethylpentene at different temperatures, the dynamic viscosity η of liquid organic compounds can be approximated on the basis of the De Guzman-Andrade equation:

$$\log\eta = B \cdot \left(\frac{1}{T} - \frac{1}{T_0}\right)$$

$\log \eta = B\ (1/T - 1/T_0)$

equates to

$$\eta = 10^{B \cdot \left(\frac{1}{T} - \frac{1}{T_0}\right)} \quad [\text{mPa·s}]$$

$\eta = 10^{B\ (1/T - 1/T0)}$ [mPa·s]

The De Guzman-Andrade equation is based on the total number of carbon atoms, not maximum chain length. 2,4,4-trimethylpentene is 5 carbons long with 8 carbons in total (n = 8). T is the Temperature [here: 40°C, 313.16K], and T_0 and B are two calculable variables (for n = number of carbon atoms ≤20; equations/ variables for ΔB_1, ΔB_2, ΔN_1, ΔN_2 and ΔN_3 are valid for alkenes with double *iso* configuration):

$T_0 = 28.86 + 37.439\ NE - 1.3547\ NE^2 + 0.02076\ NE^3$

$B = B_a + \Delta B_1 + \Delta B_2$

$B_a = 24.79 + 66.885\ NE - 1.3173\ NE^2 - 0.00377\ NE^3$

$\Delta B_1 = -44.94 + 5.410\ NE$

$\Delta B_2 = 8.93$

$NE = n + \Delta N_1 + \Delta N_2 + \Delta N_3$

$\Delta N_1 = -0.152 - 0.042\ n$

$\Delta N_2 = 1.389 - 0.238\ n$

$\Delta N_3 = 0.93$

$n = 8$

Results: NE = 7.927; B_a = 470.334; B = 477.209; T_0 = 250,854 K; η = 0.4183 mPa·s

7.1.2 Method 2 (Grain 1990):

This method is based on the normal boiling point T, the number of carbons and the compound class (Grain 1990). The viscosity at the boiling point Tb is given (0.2 mPa·s), as well as a constant K_F relating to the structure. Another parameter n does not describe the number of carbons but rather a tabulated value for the compound class.

η_B = 0.2 mPa·s (table 22-3, Grain 1990)

K_F = 1.01 (table 14-4, Grain 1990)

n = 8 (table 22-5, Grain 1990)

T_b = 375,66K (mean, Shell Research 1997)

R = 1,987 cal·mol^{-1}·K^{-1} (gas constant)

$$B_4 = \frac{1}{n} \cdot \left[K_F \cdot T_b \cdot \left(8.75 + R \cdot \ln T_b\right) - R \cdot T\right]$$

$B_4 = 1/n\ [K_F\ T_b\ (8.75 + R \ln T_b) - RT]$

$$\ln \eta = \ln \eta_B + B_4 \cdot \left(\frac{1}{T} - \frac{1}{T_b}\right)$$

$\ln \eta = \ln \eta_B + B_4\ (1/T - 1/T_b)$

$$\eta = \eta_B \cdot e^{B_4 \cdot \left(\frac{1}{T} - \frac{1}{T_b}\right)} \quad [\text{mPa·s}]$$

$\eta = \eta_B \cdot e^{B4\ (1/T - 1/Tb)}$ [mPa·s]

Results: B_4 = 886.270, ln η = -1.1386, η = 0.0735 mPa·s

1cp = 1mPa·s = 0.01 g·s^{-1}·cm^{-1}

REFERENCES

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