



**Substance Name(s): 2,2'-dichloro-4,4'-methylenedianiline**  
**EC Number: 202-918-9**  
**CAS Number: 101-14-4**

**MEMBER STATE COMMITTEE  
SUPPORT DOCUMENT FOR IDENTIFICATION OF**

**2,2'-DICHLORO-4,4'-METHYLENEDIANILINE**

**AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS  
CMR<sup>1</sup> PROPERTIES**

**Adopted on 24 November 2011**

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<sup>1</sup> CMR = carcinogenic, mutagenic or toxic for reproduction

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**Substance Name(s): 4,4'-methylenebis[2-chloroaniline];  
2,2'-dichloro-4,4'-methylenedianiline;  
MOCA**

**EC Number(s): 202-918-9**

**CAS number(s): 101-14-4**

- The substance is identified as substance meeting the criteria of Article 57 (a) of Regulation (EC) 1907/2006 (REACH) owing to its classification as carcinogen 1B<sup>2</sup> which corresponds to classifications as carcinogen category 2<sup>3</sup>.

**Summary of how the substance meets the criteria as category 1B carcinogen.**

2,2'-dichloro-4,4'-methylenedianiline (MOCA) is covered by index number 612-078-00-9 of Regulation (EC) No 1272/2008 in Annex VI, Part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances) as carcinogen, Carc. 1B (H350: "May cause cancer"). The corresponding classification in Annex VI, Part 3, Table 3.2 (the list of harmonised and classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is carcinogen, Carc. Cat. 2, R45 ("May cause cancer").

Therefore, this classification of the substance in Regulation (EC) No 1272/2008 shows that it meets the criteria for classification as carcinogen in accordance with Article 57 (a) of REACH.

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

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<sup>2</sup> 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.

<sup>3</sup> 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

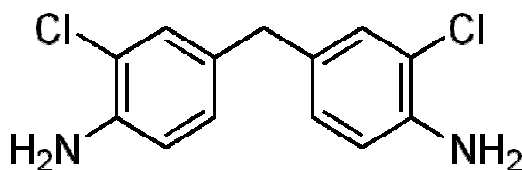
### 1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

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

**Table 1: Substance identity**

<b>EC number:</b>	202-918-9
<b>EC name:</b>	4,4'-methylenebis[2-chloroaniline]
<b>CAS number (in the EC inventory):</b>	101-14-4
<b>CAS number:</b> <b>Deleted CAS numbers:</b>	101-14-4 29371-14-0; 51065-07-7; 78642-65-6; 126699-69-2; 142661-36-7
<b>CAS name:</b>	Benzenamine, 4,4'-methylenebis[2-chloro-
<b>IUPAC name:</b>	4,4'-Methylenebis(2-chloroaniline)
<b>Index number in Annex VI of the CLP Regulation</b>	612-078-00-9
<b>Molecular formula:</b>	C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub>
<b>Molecular weight range:</b>	267.2 g/mol
<b>Synonyms:</b>	Bisamine A 2,2'-Dichloro-4,4'-methylenedianiline 3,3'-Dichloro-4,4'-diaminodiphenylmethane Bis(4-amino-3-chlorophenyl)methane

#### Structural formula:



#### 1.2 Composition of the substance

**Name:** 4,4'-Methylenebis(2-chloroaniline)

**Description:** ---

**Degree of purity:** 85 - 100 %

**Table 2: Constituents**

Constituents	Typical concentration	Concentration range	Remarks
4,4'-Methylenebis(2-chloroaniline)		85 - 100 %	Based on the information submitted in the registration dossiers

**Table 3: Impurities**

Impurities	Typical concentration	Concentration range	Remarks
Confidential information			Based on the information submitted in the registration dossiers

**Table 4: Additives**

Additives	Typical concentration	Concentration range	Remarks
None			Based on the information submitted in the registration dossiers

### 1.3 Physicochemical properties

**Table 5: Overview of physicochemical properties**

Property	Value	Reference
Physical state at 20°C and 101.3 kPa	Solid colourless crystals	Bornscheuer, U.& Roempp, 2008
Melting/freezing point	110 °C	Bornscheuer, U. & Roempp, 2008
Boiling point	Decomposing prior boiling at 370 °C	D. S. Brassington, 2010
Vapour pressure	0.0017 hPa at 60 °C	Bornscheuer, U. & Roempp, 2008
Density	1.44 g/cm <sup>3</sup> at 24 °C	Bornscheuer, U. & Roempp, 2008
Water solubility	13.8 mg/l at 20 °C; pH = 7.6	Baltussen, 2010
Partition coefficient n-octanol/water (log value)	2.5 at 25 °C and pH ca. 7	Baltussen, 2010

## 2 HARMONISED CLASSIFICATION AND LABELLING

MOCA is covered by Index number 612-078-00-9 in Annex VI, part 3 of Regulation (EC) No 1272/2008 as follows:

**Table 6: 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)		
612-078-00-9	2,2'-dichloro-4,4'-methylenedianiline; 4,4'-methylene bis(2-chloroaniline)	202-918-9	101-14-4	Carc. 1B Acute Tox. 4 * Aquatic Acute 1 Aquatic Chronic 1	H350 H302 H400 H410	GHS08 GHS07 GHS09 Dgr	H350 H302 H410			

Carc. 1B, H350	May cause cancer.
Acute Tox. 4, H302	Harmful if swallowed.
Aquatic Acute 1 H400	Very toxic to aquatic life.
Aquatic Chronic 1 H410	Very toxic to aquatic life with long lasting effects.

**Table 7: 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
612-078-00-9	2,2'-dichloro-4,4'-methylenedianiline; 4,4'-methylene bis(2-chloroaniline)	202-918-9	101-14-4	Carc. Cat. 2; R45 Xn; R22 N; R50-53	T; N R: 45-22-50/53 S: 53-45-60-61		E

Carc. Cat. 2; R45	May cause cancer.
Xn - 22	Harmful if swallowed.
N; R50-53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

### **3 ENVIRONMENTAL FATE PROPERTIES**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57a.*

A QSAR model run with default values of EPISUITE 4.00 (ECHA, 2011b) shows that MOCA is mainly sorbed to soil. However, relevant amounts of MOCA are also present in the water compartment, e.g. when equal amounts are emitted to air, water and soil still about 8 % of the substance are calculated to partition to the aquatic environment.

### **4 HUMAN HEALTH HAZARD ASSESSMENT**

*See section 2 on harmonised classification and labelling of the substance.*

### **5 ENVIRONMENTAL HAZARD ASSESSMENT**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57a.*

### **6 CONCLUSIONS ON THE SVHC PROPERTIES**

#### **6.1 PBT, vPvB assessment**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57a.*

Based on information provided in the registrations (ECHA, 2011a) it is concluded that MOCA is not readily biodegradable. This was confirmed by a QSAR study with several models (ECHA, 2011b), where a calculation with CATALOGIC (using the BIOWIN module of EPISUITE v4.00 and the 28 days aerobic biodegradation model (MITI 301C) predicted a half life for primary degradation (first degradation step) of 19 months and a half life for mineralisation of more than 10 years. The Level III fugacity model from EPISUITE 4.00, based on the default values of the model, provided half lives of 60 d, 120 d and 540 d for water, soil and sediment, respectively. 3.3 h was calculated as half life in air. It appears that the substance would meet the persistent or very persistent criteria of Annex XIII REACH.

The registrant concluded from experiments and results obtained with the OECD QSAR toolbox, that the BCF values are between 173 and 398 L/kg (ECHA, 2011a). This is in accordance with the results of the QSAR study mentioned above, in which BCF values of 176 L/kg, 234 L/kg and a maximum BCF value of 396 L/kg were calculated. This shows that MOCA has a slight tendency to bioaccumulate but does not meet the numerical B criterion of Annex XIII with a threshold of 2000 L/kg for the BCF.

The T criterion of Annex XIII is in any case fulfilled due to the harmonised classification of the substance as carcinogen (see Table 6 and Table 7). However the substance is as well very toxic to aquatic organisms with a lowest NOEC for aquatic invertebrates of 9.5 µg/L (ECHA, 2011a).

Summarising, although MOCA fulfils the T criteria of Annex XIII and appears to have persistent or very persistent properties it seems not to bioaccumulate; hence it is considered to not fulfil the PBT criteria.

## **6.2 CMR assessment**

Pursuant to Regulation (EC) No 1272/2008, MOCA is listed as entry 612-078-00-9 in Annex VI, part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008 as carcinogen category 1B<sup>1</sup>. Its corresponding classification in Annex VI, part 3, Table 3.2 (the list of harmonised and classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is carcinogen category 2<sup>2</sup>.

Therefore, this classification of 2,2'-dichloro-4,4'-methylenedianiline in Regulation (EC) No 1272/2008 shows that the substance meets the criteria for classification as carcinogen, in accordance with Article 57 (a) of REACH.

## **6.3 Substances of equivalent level of concern assessment**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57a.*



## 7 REFERENCES

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