Substance name: 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol [1]

EC number: 209-218-2
CAS number: 561-41-1

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF

4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol

[with ≥ 0.1% of Michler's ketone (EC No. 202-027-5) or Michler's base (EC No. 202-959-2)]

AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR[2] PROPERTIES

Adopted on 7 June 2012

[1] The substance is identified as SVHC only where it contains Michler's ketone (EC Number: 202-027-5) or Michler's base (EC Number: 202-959-2) ≥ 0.1% (wt/wt)

[2] CMR means carcinogenic, mutagenic or toxic for reproduction

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TABLES

Substance Name(s): 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol)[3]

EC Number(s): 209-218-2

CAS Number(s): 561-41-1

- The substance is identified as substance meeting the criteria of Article 57 (a) of Regulation (EC) 1907/2006 (REACH) where it contains Michler's ketone (EC Number: 202-027-5) or/and Michler's base (EC Number: 202-959-2) ≥ 0.1%, owing to its classification as carcinogen category 1B[4] which corresponds to classification as carcinogen category 2[5].

Summary of how the substance meets the Carcinogen 1B criteria

Michler's ketone (4,4'-bis(dimethylamino)benzophenone; EC Number: 202-027-5) is listed as Index number 606-073-00-0 in Regulation (EC) No 1272/2008 (the CLP Regulation) and classified in Annex VI, part 3, Table 3.1 (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 classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of the CLP Regulation is carcinogen, Carc. Cat. 2, R45 ("May cause cancer.")

Michler's base (N,N,N',N'-tetramethyl-4,4'-methylenedianiline; EC Number: 202-959-2) is listed as Index number 612-201-00-6 in the CLP Regulation and classified in Annex VI, part 3, Table 3.1 as carcinogen, Carc. 1B (H350: "May cause cancer.") The corresponding classification in Annex VI, part 3, Table 3.2 of the CLP Regulation is carcinogen, Carc. Cat. 2, R45 ("May cause cancer.")

According to Article 10(1) of the CLP Regulation, specific concentration limits and generic concentration limits are limits assigned to a substance indicating a threshold at or above which the presence of that substance in another substance (or in a mixture) as an identified impurity, additive or individual constituent leads to the classification of the substance (or mixture) as hazardous.

For Michler's ketone and Michler's base no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining classification of substances (or mixtures) containing Michler's ketone and/or Michler's base. The generic concentration limit for carcinogens, Carc. 1B is 0.1%, as set out in Table 3.6.2 in Part 3 of Annex I to the CLP Regulation.

Therefore, the above classifications of Michler's ketone and Michler's base in Regulation (EC) No 1272/2008 show that where 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) contains Michler's ketone or Michler's base ≥ 0.1%, it meets the criteria for classification as carcinogen in accordance with Article 57 (a) of REACH.

Registration dossiers submitted for the substance: No

[3] The substance is identified as SVHC only where it contains Michler's ketone (EC Number: 202-027-5) or Michler's base (EC Number: 202-959-2) ≥ 0.1% (wt/wt)

[4] 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.

[5] 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

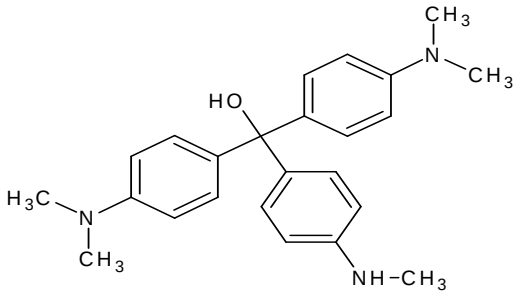
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	209-218-2
EC name:	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol
CAS number (in the EC inventory):	561-41-1
CAS number:	561-41-1
CAS name:	Benzenemethanol, α,α-bis[4-(dimethylamino)phenyl]-4-(methylamino)-
IUPAC name:	Bis[4-(dimethylamino)phenyl][4-(methylamino)phenyl]methanol
Index number in Annex VI of the CLP Regulation	
Molecular formula:	C_{24} H_{29} N_3 O
Molecular weight range:	375.5 g/mol
Synonyms:	The information is derived from the C&L notification received. Some notifiers indicated as a synonym of the substance Solvent Violet 8. However the Colour Index International identifies Solvent Violet 8 with the CAS numbers 52080-58-7 and 67989-22-4 as well with the EC number 268-006-8 which does not match the numerical identifiers with which the substance is notified.

Structural formula:



1.2 Composition of the substance

Name: 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol

Description: ---

Degree of purity: see confidential Annex

Table 2: Constituents

Constituents	**Typical concentration**	**Concentration range**	**Remarks**
4,4'-bis (dimethylamino)-4''-(methylamino)trityl alcohol EC #: 209-218-2		Confidential information	Information from C&L notifications

Table 3: Impurities

Impurities	**Typical concentration**	**Concentration range**	**Remarks**
4,4'-bis(dimethylamino)benzophenone EC #: 202-027-5		Confidential information	Information derived from the C&L notifications
N,N,N',N'-tetramethyl-4,4'-methylenedianiline EC #: 202-959-2		Confidential information	Information derived from the C&L notifications
Further impurities: Confidential information			Information derived from the C&L notifications

Table 4: Additives

Additives	**Typical concentration**	**Concentration range**	**Remarks**
None			Information derived from the C&L notifications

1.3 Physico-chemical properties

Table 5: Overview of physicochemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	solid	
Boiling point	575.3 °C at 1013 hPa	Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)
Vapour pressure	6 x 10^{-11} Pa at 25 °C	Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)
Water solubility at 25 °C	1.8 g/l at pH 4 1.7 mg/l at pH 7 1.5 mg/l at pH 9	Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)
Partition coefficient n-octanol/water (log value)	3.926 at 25 °C	Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)
Density at 20 °C	1.152 gcm^{-3}	Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2012 ACD/Labs)

2 HARMONISED CLASSIFICATION AND LABELLING

4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) is not itself listed in Annex VI of Regulation (EC) No 1272/2008.

However, according to Article 10(1) of the CLP Regulation, specific concentration limits and generic concentration limits are limits assigned to a substance indicating a threshold at or above which the presence of that substance in another substance (or in a mixture) as an identified impurity, additive or individual constituent leads to the classification of the substance (or mixture) as hazardous.

For Michler's ketone and Michler's base no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining classification of substances (or mixtures) containing Michler's ketone and/or Michler's base. The generic concentration limit for carcinogens, Carc. 1B is 0.1%, as set out in Table 3.6.2 in Part 3 of Annex I to the CLP Regulation.

4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) with Michler's ketone ≥ 0.1%

Therefore, on such basis, the classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's ketone ≥ 0.1% (wt/wt) is as follows:

Table 6: *Classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's ketone ≥ 0.1% according to Art. 10 and Table 3.6.2 in Part 3 of Annex I to Regulation (EC) No 1272/2008 (CLP Regulation), on the basis of the entry with index number 606-073-00-0 in Part 3 of Annex VI to CLP Regulation, Table 3.1*

Substane name	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 state-ment code(s)	Suppl. Hazard statement code(s)		
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol)with Michler's ketone ≥ 0.1%	209-218-2	561-41-1	Carc. 1B Muta. 2 Eye Dam. 1	H350 H341 H318	GHS08 GHS05 Dgr	H350 H341 H318	-	-	-

Table 7: *Classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's ketone ≥ 0.1% according to Art. 10 and Table 3.6.2 in Part 3 of Annex I to Regulation (EC) No 1272/2008 (CLP Regulation), on the basis of the entry with index number 606-073-00-0 in Part 3 of Annex VI to CLP Regulation, Table 3.2*

Substance name	EC No	CAS No	Classification	Labelling	Concentration Limits	Notes
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) with Michler's ketone ≥ 0.1%	209-218-2	561-41-1	Carc. Cat. 2; R45 Muta. Cat. 3; R68 Xi; R41	T R: 45-41-68 S: 53-45	-	-

4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) with Michler's base ≥ 0.1%

On the same basis, the classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's base ≥ 0.1% (wt/wt) is as follows:

Table 8: *Classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's base ≥ 0.1% according to Art. 10 and Table 3.6.2 in Part 3 of Annex I to Regulation (EC) No 1272/2008 (CLP Regulation), on the basis of the entry with index number 612-201-00-6 in Part 3 of Annex VI to CLP Regulation, Table 3.1*

Substane name	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 state-ment code(s)	Suppl. Hazard statement code(s)		
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) with Michler's base ≥ 0.1%	209-218-2	561-41-1	Carc. 1B Aquatic Acute 1 Aquatic Chronic 1	H350 H400 H410	GHS08 GHS09 Dgr	H350 H410	-	-	-

Table 9: *Classification of 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) where it contains Michler's base ≥ 0.1% according to Art. 10 and Table 3.6.2 in Part 3 of Annex I to Regulation (EC) No 1272/2008 (CLP Regulation),, on the basis of the entry with index number 612-201-00-6 in Part 3 of Annex VI to CLP Regulation, Table 3.2*

Substance name	EC No	CAS No	Classification	Labelling	Concentration Limits	Notes
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) with Michler's base ≥ 0.1%	209-218-2	561-41-1	Carc. Cat. 2; R45 N; R50-53	T; N R: 45-50/53 S: 53-45-60-61	-	-

3 ENVIRONMENTAL FATE PROPERTIES

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

4 HUMAN HEALTH HAZARD ASSESSMENT

See section 2 on harmonised classification and labelling.

5 ENVIRONMENTAL HAZARD ASSESSMENT

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

6 CONCLUSIONS ON THE SVHC PROPERTIES

6.1 CMR Assessment

Michler's ketone (4,4'-bis(dimethylamino)benzophenone; EC Number: 202-027-5) is listed as Index number 606-073-00-0 in Regulation (EC) No 1272/2008 (the CLP Regulation) and classified in Annex VI, part 3, Table 3.1 (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 classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of the CLP Regulation is carcinogen, Carc. Cat. 2, R45 ("May cause cancer.")

Michler's base (N,N,N',N'-tetramethyl-4,4'-methylenedianiline; EC Number: 202-959-2) is listed as Index number 612-201-00-6 in the CLP Regulation and classified in Annex VI, part 3, Table 3.1 as carcinogen, Carc. 1B (H350: "May cause cancer.") The corresponding classification in Annex VI, part 3, Table 3.2 of the CLP Regulation is carcinogen, Carc. Cat. 2, R45 ("May cause cancer.")

According to Article 10(1) of the CLP Regulation, specific concentration limits and generic concentration limits are limits assigned to a substance indicating a threshold at or above which the presence of that substance in another substance (or in a mixture) as an identified impurity, additive or individual constituent leads to the classification of the substance (or mixture) as hazardous.

For Michler's ketone and Michler's base no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining classification of substances (or mixtures) containing Michler's ketone and/or Michler's base. The generic concentration limit for carcinogens, Carc. 1B is 0.1%, as set out in Table 3.6.2 in Part 3 of Annex I to the CLP Regulation.

Therefore, the above classifications of Michler's ketone and Michler's base in Regulation (EC) No 1272/2008 show that where the substance 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol) contains Michler's ketone or Michler's base ≥ 0.1% it meets the criteria for classification as carcinogen in accordance with Article 57 (a) of REACH.