

Summary of Initial Risk Assessment Report

3,3'-Dichloro-4,4'-diaminodiphenylmethane CAS No : 101-14-4

PRTR No of Japan: 120

This substance is assessed based on Guideline for Initial Risk Assessment Version 1.0

1. General Information

1.1 Physico-chemical properties

Appearance	Colorless solid
Melting point	110 degC
Boiling point	None (degradable at 200 degC or above)
Water solubility	13.9 mg/L (24 degC)
Henry's constant	$4.11 \times 10^{-6} \text{ Pa} \cdot \text{m}^3/\text{mol}$ ($4.06 \times 10^{-11} \text{ atm} \cdot \text{m}^3/\text{mol}$) (25degC, estimated)
Octanol/water partition coefficient (log Kow)	3.91 (measured), 3.47 (estimated)
Soil adsorption coefficient	$K_{oc} = 1.4 \times 10^4$ (estimated)

1.2 Environmental fate

Bioaccumulation	Exhibits little to no bioaccumulation Bioconcentration factor (BCF) : 130-398 (50 microg/L), 114-232 (5 microg/L) (carp), (measured)
Biodegradation	Non-biodegradable
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is $7.8 \times 10^{-11} \text{ cm}^3/\text{molecule} \cdot \text{sec}$. (25 degC, estimated) The half-life is 3-5 hours, given OH radical concentration of $5 \times 10^5 - 1 \times 10^6 \text{ molecule}/\text{cm}^3$. Reaction with ozone: No data Reaction with nitrate radical: No data 3,3'-Dichloro-4,4'-diaminodiphenylmethane (hereinafter referred to as "MBOCA") may be directly degraded by photolysis. (In water) MBOCA is expected to be photodegradable in surface water. Hydrolysis is not expected to occur in the aquatic environment, since MBOCA lacks functional groups that hydrolyze under environmental conditions.
Environmental fate	If released into water, MBOCA is expected to be adsorbed to suspended solids in water and transferred to sediments. Removal from water by volatilization to air is not considered to be an important fate process.

2. Sources of release to the environment

2.1 Annual production, import, export and domestic supply in 2001 (ton/year)

Production	Import	Export	Domestic supply	Remarks
4,000	--	--	--	

2.2 Uses

Curing agents for urethane resin (waterproof materials, flooring materials, and all-weather pavement materials)

2.3 Release from the industries within the scope of PRTR system (in 2001)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	< 0.5	< 0.5	0	Release to rivers: 1.08 tons
	Release outside notification	7	1	0	
Release outside notification from non listed industry		--	--	--	
Households		--	--	--	
Mobile sources		--	--	--	
Total		7	1	0	

2.4 Releases from other sources

No information about the substance is available.

2.5 Main release route

MBOCA is expected to be released into the environment mainly during use of MBOCA and products containing it.

3. Exposure Assessment

3.1 Measured environmental concentration

Media	No. of points detected / No. of points measured	No. of samples detected / No. of samples measured	Detection range	95th percentile	Detection limit	Year of investigation, Institution
Air	No data	--	--	--	--	--
River water (microg/L)	--	0/30	nd	--	5	1985 Ministry of the Environment
Drinking water	No data	--	--	--	--	--
Food	No data	--	--	--	--	--

nd: Not detected

3.2 Estimated environmental concentration

Media	Estimated concentration	Description
Air (microg/m ³)	1.6×10^{-3}	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment ver.1.0 (AIST-ADMER)
River water (microg/L)	0.034	Calculated by mathematical model / Integrated River Model to predict the distribution of chemical concentration (IRM1)

3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	0.034
	Estimated concentration by model (0.034 microg/L) was used for the risk assessment, since adequate measured data was not available ¹⁾ .

3.4 Estimated human intake

Intake route		Concentration used for estimation of intake	Estimated intake (microg/ person/ day)	Estimated intake (microg/ kg-Bodyweight (BW)/ day)
Inhalation	Air	0.0016 (microg/m ³)	0.032	0.00064
		Estimated concentration (1.6*10 ⁻³ microg/m ³) was used, since measured concentration was not available.		
Oral	Drinking water	0.034 (microg/L)	0.068	0.00136
		-Concentration in river water was used as a substitute for that in drinking water, since measured concentrations in tap water nor ground water were not available. -Estimated concentration in river water by model was used, since measured concentration in river water is outdated.		
	Food	0.0014 (microg/g)	0.16	0.0032
		-No data on food were available. - The concentration in fish was calculated as a product of a concentration in sea water and a BCF. -Concentrations in seawater were estimated as one-tenth of the estimated concentration in river water. 0.034 (microg/L) (estimated river water concentration) * 1/10 * 398 (L/kg) = 1.4 (microg/g)		
Subtotal	--	0.23	0.0046	
Total route		--	0.26	0.0052

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version 1.0. If adequate measured concentrations are available, they are given priority and used as values for risk assessment. If they are not available, an estimated value calculated using a mathematical model is used.

4. Hazard assessment

4.1 Effects on organisms in the environment

	Acute or Chronic	Species	Endpoint	Concentration
Algae	Chronic	<i>Selenastrum capricornutum</i>	96 hours NOEC Growth inhibition (biomass)	0.313 (mg/L)
Crustacea	Chronic	<i>Daphnia magna</i>	21 days NOEC Reproduction, mortality of parents	0.0375 (mg/L)
Fish	Acute	<i>Oryzias latipes</i>	96 hours LC ₅₀	0.657 (mg/L)
Key study		The toxic data of crustacea (<i>daphnia magna</i>) was chosen for the key study because effects were observed at the lowest concentration in the hazard assessment.		

4.2 Human health toxicity

Toxicity	Exposure route	Species	Duration / Dose method	Toxic effects (Key study is underlined)	NOAEL or LOAEL
Repeated dose toxicity	Inhalation		No data	--	--
	Oral		No data	--	--
	Dermal		No data	--	--
Reproductive and developmental toxicity	--		No data	--	--
Carcinogenicity	Evaluation by IARC : Group 2A (Probably carcinogenic to humans)				
Genotoxicity	Considered to be genotoxic				

5. Risk Assessment

5.1 Environmental organisms

Risk characterization	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
	0.034	NOEC: 0.0375	1,100	50	No immediate concern
Product of uncertainty factors (UF): Extrapolation from laboratory test (10) * Toxicity data on two nutritional stages (5) = 50					
Recommendation : The substance is considered to be of no immediate concern for the moment, and a low priority for further work.					

* NOEC means NOEC, LOEC, EC₅₀, etc.

5.2 Human health

5.2.1 Repeated dose toxicity

Exposure route	Intake (microg/kgBW/day)	NOAEL (mg/kgBW/day)	Risk characterization		
			MOE	Product of uncertainty factors	Conclusion
Inhalation	0.00064	No data	--	--	--
Oral	0.0046		--	--	--
Total	0.0052		--	--	--
Product of uncertainty factors (UF): --					

5.2.2 Reproductive and developmental toxicity

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5.2.3 Carcinogenicity

Risk characterization of carcinogenicity of the substance was not carried out in this assessment.

5.2.4. Recommendation for Human Health

The substance could not be assessed because no adequate data were available. It should be noted that a carcinogenic risk characterization was not conducted. The possibility remains that this substance may be carcinogenic to humans.

6. Supplement

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