Canadian Environmental Protection Act

Priority Substances List

Supporting Documentation - Environmental Sections

3,5-DIMETHYLANILINE

(Unedited Version)

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1.0 Identity of substance

1.1 Name of substance

3,5-Dimethylaniline (Chemical Abstracts Service Registry Number 108-69-0) is one of six isomeric dimethylanilines, or xylidines, with a molecular formula of $C_8H_{11}N$. Its structure is shown in Fig. 1. Synonyms for 3,5-dimethylaniline include 3,5-xylidine, 3,5-dimethylphenylamine, 3,5-dimethylbenzamine and 1-amino-3,5-dimethylbenzene.

1.2 Characteristics of substance

3,5-Dimethylaniline is a pale to yellow oily liquid at room temperature (Weast *et al.,* 1984).

1.3 Analytical methodology

3,5-Dimethylaniline in water, sediments and tissues can be determined by standard techniques of extraction and gas chromatography, *e.g.,* the U.S. Environmental Protection Agency base/neutral method (U.S. Environmental Protection Agency, 1984). Detection limits will depend upon the detector used. No data were identified on detection limits for 3,5-dimethylaniline.

2.0 Physical and chemical properties

Table 1 gives the physical and chemical properties of 3,5-dimethylaniline. The vapour pressure and aqueous solubility have not been determined. Estimated values are: a vapour pressure of 7.4 Pa at 25°C (calculated according to Method 1 described by Grain (1982)), and a water solubility of 248.5 mg/L at 25°C (calculated according to Kenaga and Goring (1980)). Reported values for the octanol-water partition coefficient are 2.21 (calculated using CLOGP version 3.3 - Newsome *et al.*, 1987) and 3.04 (measured - Tonogai *et al.,* 1982).

3.0 Sources and releases to the environment

3.1 Natural sources

No natural sources of 3,5-dimethylaniline have been identified.

3.2 Anthropogenic sources

3.2.1 Production and market trends

Production of 3,5-dimethylaniline in the U.S.A in 1986 was 19.2 tonnes, and none was produced in 1990 (U.S. Environmental Protection Agency, 1992). No other information was identified on market trends.

3.2.2 Canadian consumption, imports and exports

3,5-Dimethylaniline is not produced in Canada or imported into Canada (Canada Department of Environment, 1990, 1991a,b). No information was identified on its incorporation into products imported into Canada.

3.2.3 Manufacturing processes

3,5-Dimethylaniline can be produced by the reduction of 3,5-dimethylnitrobenzene with iron in strong acid (Sandridge and Staley, 1978).

3.2.4 Uses

3,5-Dimethylaniline and other xylidine isomers are mainly used as intermediates in the manufacture of azo dyes (Northcott, 1978; Budavari, 1989). It is also used in the manufacture of pharmaceuticals, curing agents, antioxidants and antiozonants, gasoline additives and detergents, wood preservatives, wetting agents for textiles, frothing agents for ore dressing, special lacquers and metal complexers.

3.2.5 Releases

3,5-Dimethylaniline can, in principle, enter the environment from any stage in the production, storage, transport, use, disposal, or environmental degradation of 3,5-dimethylaniline itself or 3,5-dimethylaniline-containing materials such as azo dyes, or by atmospheric and water-borne transport from other countries. It may be produced in various coal conversion processes (Schultz *et al.*, 1978), but there is no information on the releases of this compound to the environment in Canada. It could also be produced by the reduction in aquatic environments of 3,5-dimethylnitrobenzene, but there is no information on releases of this compound to the environment in Canada or elsewhere. There is no indication of transboundary transport. No information was found in the literature on effluent or emission data on 3,5-dimethylaniline in Canada or other countries. Therefore, no sources or releases of 3,5-dimethylaniline into Canada have been identified.

4.0 Environmental transport, transformation and concentrations

4.1 Transport and distribution between and within media

There are not enough measured physical and chemical data and degradation rate constants on 3,5-dimethylaniline to allow an estimate to be made of the relative importance of various pathways of distribution.

4.1.1 Water

Based on the estimated vapour pressure and aqueous solubility of 3,5-dimethylaniline, the half-life for its volatilization from surface waters (1 m deep, flowing at 1 m/s, with wind velocity of 3 m/s) to the atmosphere at 20 °C was estimated to be 29.5 h (according to a method described by Thomas (1982)), which indicates that it is a low-to-medium volatility compound as far as volatilization from water is concerned.

The pK_a value of 4.89 for 3,5-dimethylaniline (Perrin, 1965) indicates that more of this chemical will be ionized at environmental pH values than is the case for aniline (pK_a 4.63 - Weast *et al.,* 1984). This may make binding to clays relatively more important compared to binding to soil organic matter.

4.1.2 Soil

The measured value of 3.04 for the log (octanol-water partition coefficient) of 3,5-dimethylaniline (Tonogai *et al.*, 1982) indicates some potential for binding to soil. However, no soil-binding studies were identified.

4.1.3 Biota

The measured value of 3.04 for the log (octanol-water partition coefficient) of 3,5-dimethylaniline (Tonogai *et al.*, 1982) indicates some potential for bioaccumulation. However, no bioaccumulation studies were identified.

4.2 Transformation

There are not enough measured physical and chemical data and degradation rate constants on 3,5-dimethylaniline to allow an estimate to be made of the relative importance of various pathways of transformation. By analogy with aniline (which is also on the CEPA Priority Substances List and which is being assessed separately) it is anticipated that 3,5-dimethylaniline will be relatively non-persistent in the environment and that biological degradation will be a major process determining its persistence in the aquatic and soil environments.

4.2.1 Biodegradation

Only one report was identified on the environmental persistence of 3,5-dimethylaniline. Baird *et al.* (1977) showed that 3,5-dimethylaniline was degraded by activated sludge about as quickly as aniline, *i.e.,* with a half-life of hours to days.

4.2.2 Abiotic degradation

By analogy with aniline, sunlight photolysis of 3,5-dimethylaniline may be important in water and on soil. It is anticipated that sunlight photolysis will be important in air. Because 3,5-dimethylaniline is of low-to-medium volatility, and because it is expected to photolyze readily in air, it is not expected to contribute to phenomena such as ozone depletion, global warming or the formation of ground-level ozone.

4.3 Environmental concentrations

No information was identified on 3,5-dimethylaniline or other xylidine concentrations in surface water, groundwater, air, soil, sediment or biota in Canada or elsewhere.

5.0 Population exposures

Refer also to supporting documentation from Health and Welfare Canada.

5.1 Exposures of wildlife populations

No data were identified for the exposure of 3,5-dimethylaniline to wild mammals, terrestrial organisms, birds, sediment or soil biota in Canada or elsewhere.

5.2 Exposures of the general human population

Refer to supporting documentation from Health and Welfare Canada.

6.0 Toxicokinetics and metabolism

Refer to supporting documentation from Health and Welfare Canada.

7.0 Mammalian toxicology

Refer to supporting documentation from Health and Welfare Canada.

8.0 Effects on humans

Refer to supporting documentation from Health and Welfare Canada.

9.0 Effects on the ecosystem

9.1 Aquatic toxicity

Little information was identified on the toxic effects of 3,5-

dimethylaniline. Tonogai *et al.* (1982) found 24-h and 48-h LC_{50} values of 35 and 17 mg/L, respectively, for medaka (*Oryzias latipes*). Baird *et al.* (1977) have shown that 3,5-dimethylaniline at 20 mg/L had some inhibitory effect on the respiration of organisms in activated sludge even while being degraded, which suggests that a metabolite or metabolites may be responsible for the observed toxicity. Kaiser and Palabrica (1991) found EC_{50} values of 14-19 mg/L for light output in a bacterium, *Photobacterium phosphoreum*. Schultz *et al.* (1978) found a 48-h LC_{100} value of 273 mg/L for a ciliate, *T. pyriformis*. Using a quantitative structure-activity relation approach, Kaiser (1992) has estimated the following 96-h LC_{50} values: 22 mg/L for fathead minnow (*Pimephelas promelas*), 11 mg/L for rainbow trout (*Oncorhynchus mykiss*), and 14 mg/L for golden orfe (*Leuciscus idus melanotus*).

No data were identified on the chronic toxicity of 3,5-dimethylaniline to aquatic organisms.

9.2 Terrestrial toxicity

No data were identified for the acute or chronic toxicity of 3,5-dimethylaniline to wild mammals, terrestrial organisms, birds, sediment or soil biota.

10.0 References

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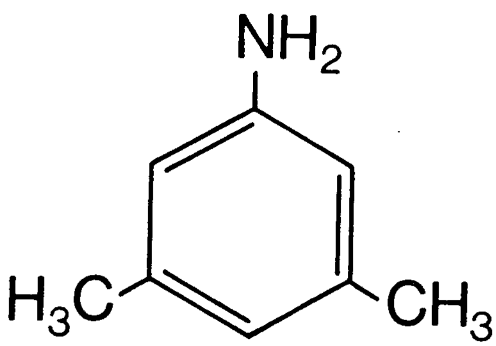
Table 1. Chemical and physical properties of 3,5-dimethylaniline

Property		Reference
molecular formula	$C_8H_{11}N$	
molecular weight	121.18	
appearance	pale to yellow oily liquid	Weast *et al.* (1984)
melting point	9.8 °C	Weast *et al.* (1984)
boiling point	220 °C	Weast *et al.* (1984)
density	0.97 g/cm^3	Weast *et al.* (1984)
refractive index	1.5581	Weast *et al.* (1984)
pK_a	4.89	Perrin (1965)
log (octanol-water partition coefficient)	2.21	Newsome *et al.* (1987)
	3.04	Tonogai *et al.* (1982)

Figure 1. Chemical structure of 3,5-dimethylaniline.



3,5-DIMETHYLANILINE