

SIDS Initial Assessment Report

for

11th SIAM

(USA, January 23-26, June 2001)

Chemical Name: Dipropylene glycol, mixed isomers and dominant isomer

CAS No: 25265-71-8 and 110-98-5

Sponsor Country: U.S.A

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HISTORY: At SIAM 11 the recommendation of Low Priority for Further Work was agreed. Revisions to the SIAR and preparation of Robust Summaries were requested and agreed.

COMMENTS:

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Dipropylene Glycol SIAR

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Chapter 1. Identity

Commercial dipropylene glycol (CAS # 25265-71-8; $(\text{CH}_3\text{-CHOH-CH}_2\text{O-CH}_2\text{-CHOH-CH}_3)$) is composed of 3 isomers (2,2'-dihydroxydiisopropylether (CAS-No.: 108-61-2); 2,2'-dihydroxydipropylether (CAS-No.: 110-98-5); 2-hydroxypropyl-2'-hydroxyisopropyl-ether (CAS-No.: 106-62-7) and is typically 98% pure. It is a liquid that possesses the following physico-chemical properties and characteristics:

Property	Value
Chemical Formula	$(\text{CH}_3\text{CHOCH}_2)_2\text{O}$
Molecular Weight	134.2
Purity	$\geq 98\%$ w/w
Impurities	
Solubility	Miscible with water
Melting Point	$< -39\text{ }^\circ\text{C}$
Boiling Point	$222.2 - 236\text{ }^\circ\text{C}$
Density	1022-1025 mg/ml at $20\text{ }^\circ\text{C}$
Vapor Pressure	0.01 hPa at $20\text{ }^\circ\text{C}$ 0.05 hPa at $21\text{ }^\circ\text{C}$
Log Kow	-1.486
Synonyms	DPG; Di-1,2-propyleneglycol; oxybispropanol; Practical

Chapter 2. General Information on Exposure

2.1 Production

Dipropylene glycol is produced as a byproduct of the manufacture of propylene glycol. The United States (US) production capacity of dipropylene glycol (i.e., byproduct production capacities of propylene glycol plants) was 131 million pounds (60 thousand tonnes) in 1998. The US Domestic demand in 1998 was 108 million pounds (49 thousand tonnes). In 1998, dipropylene glycol was produced in the US by The Dow Chemical Company, Eastman Chemical Company, Huntsman Corporation, Lyondell Chemical Company, and Olin Corporation. (ChemExpo Chemical Profile, 1998). Worldwide capacity is estimated at 235 million pounds (107 thousand tonnes).

2.2 Use

Dipropylene glycol is used primarily as an industrial intermediate, but is also used as a substance in consumer products, and as an ingredient in pesticidal formulations. Uses of dipropylene

glycol as a substance capitalize on its superior performance as a plasticizer as well as properties (e.g., high solvency, high viscosity) that permit dipropylene glycol to act as a functional ingredient of fluids. The uses of dipropylene glycol are listed in the following table.

USES OF DIPROPYLENE GLYCOL

USES	APPLICATION	FUNCTION	% PRODUCTION
Intermediate	Specialty plasticizer	Plasticizer	38 %
Intermediate	Non-reinforced polyesters	Resin monomer	23 %
Substance	Cosmetics and Fragrances	Humectant, Emollient	10 %
Intermediate	Polyurethane polyols	Plasticizer	10 %
Intermediate	Alkyd resins	Resin monomer	7 %
Substance, Intermediate	Miscellaneous (e.g., dyes & inks, paints & coatings; functional uses in hydraulic brake fluids; cutting oils)	Solvent, functional fluid, coolant	14%

(Source: ChemExpo Chemical Profile (1998)).

The uses listed in the table above have been grouped and assigned a publicly available percentage of production. The Environmental Defense (ED) Scorecard website (Source: www.scorecard.org). for dipropylene glycol lists 6 consumer product types and 18 pesticidal products containing dipropylene glycol. Data available from the US EPA indicates that in 2001 there are two pesticidal products containing dipropylene glycol as an ingredient registered in the US, whereas 20 such products have been registered over time (Source: California Department of Pesticide Registration website, <http://www.cdpr.ca.gov/cgi-bin/epa/chemdet.pl?pccode=068604>).

2.3 Exposure

As most dipropylene glycol in the US is used in industrial applications, occupational exposures via the dermal or inhalation route present a potential for exposure. In the commercial service and consumer settings use as a functional fluid (e.g. in hydraulic brake fluids, cutting oils) or as an ingredient in pesticides present a potential for inhalation exposure in addition to dermal exposure.

In the consumer setting, dermal exposure, and to a lesser degree inhalation exposure are to be expected where dipropylene glycol is formulated into cosmetic or fragrance products.

DIPROPYLENE GLYCOL EXPOSURE POTENTIAL

POPULATION	ROUTE(S) OF EXPOSURE	SOURCE(S)
Occupational Exposure	Dermal Inhalation	Manufacturing Industrial use as Intermediate Commercial Service
Consumer	Dermal Inhalation	Cosmetics, fragrances, germicidal products

The use concentration of dipropylene glycol in branded pesticidal products is also available. This is summarized in the following table.

PESTICIDAL FORMULATIONS CONTAINING DIPROPYLENE GLYCOL

RANGE OF CONCENTRATION (%)			
	<1	1-5	>5
No. of Brand Name Products	1	16	1

(Source: EDF Website: www.scorecard.org)

Only two of the 18 branded products shown in the above table currently (May, 2001) maintain active registrations in the US, and both contain dipropylene glycol in the 1 to 5 percent range.

Exposure of dipropylene glycol from environmental sources is expected to be low. Very low levels of dipropylene glycol have been reported in drinking water (0.2 and 0.4 ng/l) and 5 paper mill waste water treatment plants effluents (11 µg/l). Because of its low volatility detection of dipropylene glycol in air samples is not expected.

Chapter 3. Environment

3.1 Environmental Exposure

Based on the available data, dipropylene glycol is expected to present a low hazard to the environment. If released into the environment, it will preferentially partition into water. Because of its low soil sorption coefficient (K_{oc}), dipropylene glycol is expected to mobilize if spilled on soil and will not adsorb to particles. Volatility is not expected to be a significant fate process for this material due to its low vapor pressure and high water solubility. Photodegradation of the material in air or water is also not expected to be a significant fate process. Once in the environment, dipropylene glycol is capable of being degraded under aerobic conditions by bacteria present in soil and water. As is typical for ethers and glycols, dipropylene glycol is hydrolytically stable. Results of the octanol/water partition coefficient (expressed as $\log K_{ow}$) and from bioaccumulation studies with carp (MITI, 1992) indicate that dipropylene glycol is not expected to significantly accumulate in aquatic organisms (BCF 0.3 to 4.6).

3.2 Environmental Partitioning

Based on the EPIWIN Level III Fugacity Model (Mackay, 1991), dipropylene glycol is expected to partition primarily to water and soil.

Compartment	Percent
Air	0.107
Water	46.1
Soil	53.7
Sediment	0.0768

The results predicted by the model are consistent with study data generated on dipropylene glycol. Based on the low soil sorption coefficient (K_{oc} 3 to 56.2), dipropylene glycol would be expected to mobilize following exposure to soil and would not bind to sediment or soil particles. Mathematical modeling of photodegradation gives an estimated atmospheric half-life of 13 hours, supporting the model results suggesting that the air compartment is not a significant fate process following release of dipropylene glycol. Hydrolysis of dipropylene glycol in water and soil is also not expected to be an important fate process.

Results from biodegradation studies show that dipropylene glycol is biodegraded in water and expected to be biodegraded in soil. Degradation (>70% in 28 days) was observed when the Zahn-Wellens test was used (BASF, 1989), but not when the same compound was evaluated in the MITI test (MITI, 1992). Differences in the technique used to add dipropylene glycol to the test flasks was an important variable in determining the potential degradation of the test substance under the conditions used in these tests. Additional biodegradation tests with *Corynebacterium* sp. under vigorous shaking conditions and with soil bacteria confirmed that dipropylene glycol is biodegradable when contact between the test substance and bacteria is enhanced (Kawai *et al.*, 1977, 1985). Evaluation of the BOD5/COD plants (Bridie *et al.*, 1979b) and the acute toxicity of dipropylene glycol to *Pseudomonas putida* (Claussen, 1993) demonstrate that dipropylene glycol is not expected to be toxic or to cause a significant oxidative load to wastewater treatment

3.3 Effects on the Environment

Based on a combination of test data, quantitative structure activity relationship analysis (QSAR), and data on analogs (propylene glycol, tripropylene glycol), dipropylene glycol presents a low hazard concern for the environment. Representative results for dipropylene glycol include:

Organism	Duration (hrs.)	LC ₅₀ /EC ₅₀ (mg/l)	Source
<u>Fish</u> <i>Carassium auratus</i>	24	>5,000	Bridie <i>et al.</i> , 1979a
<u>Amphibians</u> <i>Rana brevipoda porosa</i> <i>Xenopus laevis</i>	48 48	5,300 3,181	Nishiuchi, 1984 DeZwart and Slooff, 1987
<u>Bacteria</u> <i>Pseudomonas putida</i>	18	1,000 (EC ₁₀)	Claussen, 1993

Toxicity predictions using QSAR support the general conclusions of low toxicity. QSAR predictions for dipropylene glycol based on SARs (chemical class = alcohol ether) for neutral organic chemicals include:

Fish 96-hour LC ₅₀	>10,000 mg/l
Daphnid 48-hour LC ₅₀	>10,000 mg/l
Green algal 96-hour LC ₅₀	>10,000 mg/l
Fish chronic value (ChV)	>1,000 mg/l
Daphnid ChV	470 mg/l
Algal ChV	340 mg/l

Toxicity values for the analogs propylene glycol and tripropylene glycol also support the expected lack of aquatic toxicity, with fish LC₅₀ values of >46,000 mg/l and >1,000 mg/l, invertebrate EC₅₀ values of 10,000 mg/l and > 1,000 mg/l and aquatic plant EC₅₀ values of 19,000 mg/l and >1,000 mg/l for propylene glycol and tripropylene glycol, respectively. Although chronic study data for dipropylene glycol are not available, QSAR predictions suggest that this test substance will not cause chronic toxicity to aquatic organisms. Published studies are not available on the effects of dipropylene glycol on terrestrial organisms or plants, however, little effect is expected, since dipropylene glycol degrades in soil, has very low bioaccumulation potential, and is of low toxicity to aquatic organisms.

Based on the QSAR data for Daphnia and algal toxicity, and the measured data for fish and amphibians, dipropylene glycol is not expected to be toxic to aquatic organisms except at very high concentrations. Using an assessment factor of 100 and the goldfish (*Carassius auratus*) data (LC₅₀ >5,000 mg/l), a predicted no effect concentration (PNEC) of >50 mg/l is obtained. Using the clawed toad (*Xenopus laevis*) data (LC₅₀ 3,181 mg/l), and an assessment factor of 100, the PNEC is 32 mg/l.