

2002 SEP 12 PM 12: 25

Table 1 - Solvent C (CAS No.:68990-21-6)

Cas No.	Chemical	Composition Percentage	General Comments
10143-60-9	di-2-Ethylhexyl ether	25-35	The only data located was an LD50 that indicates it is of low toxicity (LD ₅₀ of 33.9 g/kg; Smyth, H.F., 1954). It is listed by the EPA as a Class 3 inert ingredient for use in pesticide formulations. The EPA is in the process of preparing toxicological and ecological assessments for this class level of inert ingredients.
109-21-7	Butyl butyrate	8-16	Material is an FDA-approved food flavorant and is naturally present in many types of fruits. It is fully expected to metabolize to butyric acid and n-butanol in mammals. Both these chemicals are in the ICCA HPV program.
126-30-7	Neopentyl glycol	7-11	An OECD/SIDS assessment has been completed.
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	7-11	A complete test plan with robust summaries for all end points has been submitted into the EPA as part of the HPV program.
71-36-3	n-butyl alcohol	5-10	Material is in the ICCA/SIDS program.
94-96-2	2-Ethyl-1,3-hexanediol	5-10	Material has been thoroughly characterized for use as an insect repellent for human uses. Although its registration has been cancelled, essentially all SIDS data are available through published literature.
NA	Alkyl Acetals	2-10	Formed by a reaction between alcohols and aldehydes. The reaction is readily reversed in the presence of an acid.
104-76-7	2-Ethylhexanol	4-6	An OECD/SIDS assessment has been completed.
78-83-1	Isobutyl alcohol	2-6	Material is in the ICCA/SIDS program.
97-85-8	Isobutyl isobutyrate	2-6	Material is in the ICCA/SIDS program.
107-92-6	Butyric acid	1-2	Material is in the ICCA/SIDS program.

SIDS DATA SUMMARY

Solvent C is a mixture of several chemicals, the majority of which have already been or are in the process of being evaluated in the OECD SIDS program, the ICCA SIDS program, or the US EPA HPV program. Accordingly, it should be assumed that they already have or will have complete data sets and have robust summaries available as a result of their participation in these programs. Another chemical, 2-ethyl-1,3-hexanediol, present at a level of 5-10% has data assessing all of the mammalian endpoints available to the public via peer-reviewed journals. This is the only other chemical with significant amounts of data that can be used to assist in determining the hazard potential of the mixture. However, since it only constitutes a small fraction of the total its toxicity is not likely to impact the overall toxicity in a significant manner and all data available indicate it is of low toxicity to both mammalian and environmental species. Since Solvent C consists of many chemicals present in varying amounts it is not known how the various SIDS endpoints will be affected by their presence as a mixture. Due to the fact that the actual percentage of each chemical can vary, Eastman believes there would be little value in conducting any new animal studies on Solvent C when the hazard associated with the majority of its constituents have been already assessed.

PHYSICAL CHEMICAL DATA

Cas No.	Chemical	Melting Point*	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility
10143-60-9	di-2-Ethylhexyl ether	NA	X	X	X	X
109-21-7	Butyl butyrate	NA	X	X	X	X
126-30-7	Neopentyl glycol	NA	X	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	NA	X	X	X	X
71-36-3	n-butyl alcohol	NA	X	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	NA	X	X	X	X
NA	Alkyl Acetals	NA				
104-76-7	2-Ethylhexanol	NA	X	X	X	X
78-83-1	Isobutyl alcohol	NA	X	X	X	X
97-85-8	Isobutyl isobutyrate	NA	X	X	X	X
107-92-6	Butyric acid	NA	X	X	X	X

* Material is a liquid at room temperature

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data are available through the use of computer estimation modeling programs (EPIWIN) that are available to the public.

ENVIRONMENTAL FATE

Cas No.	Chemical	Photo-degradation	Water Stability	Biodegradation	Fugacity
10143-60-9	di-2-Ethylhexyl ether	X			X
109-21-7	Butyl butyrate	X	X		X
126-30-7	Neopentyl glycol	X	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X	X
71-36-3	n-butyl alcohol	X	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X	X	X ¹	X
NA	Alkyl Acetals				
104-76-7	2-Ethylhexanol	X	X	X	X
78-83-1	Isobutyl alcohol	X	X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X	X
107-92-6	Butyric acid	X	X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data are available through the use of computer estimation modeling programs (EPIWIN) that are available to the public.

- 1.) Data (OECD 301E and 302B) listed in a MSDS from Dixie Chemical Company, Inc. Houston, TX indicate this material is readily degradable.

ECOTOXICITY DATA

Cas No.	Chemical	Fish Toxicity	Daphnia Toxicity	Algae Growth Inhibition
10143-60-9	di-2-Ethylhexyl ether			
109-21-7	Butyl butyrate	X ¹		
126-30-7	Neopentyl glycol	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X
71-36-3	n-butyl alcohol	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X ²	X ²	
NA	Alkyl Acetals			
104-76-7	2-Ethylhexanol	X	X	X
78-83-1	Isobutyl alcohol	X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X
107-92-6	Butyric acid	X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data could be generated through the use of computer estimation models that are available to the public.

- 1.) Curtis, M.W. and Ward C.H. (1981). Aquatic Toxicity of Forty Industrial Chemicals: Testing in Support of Hazardous Substance Spill Prevention Regulation. *J Hydrology*, **51**, 359-367.
- 2.) Data (LC0(48hr) Fish > 1000 mg/L; EC50(24 hr) Daphnia 811 mg/L) listed in a MSDS from Dixie Chemical Company, Inc. Houston , TX

TOXICOLOGICAL DATA

Cas No.	Chemical	Acute Toxicity	Repeat Dose Toxicity	Genotoxicity Mut./Aberr.	Developmental Toxicity	Reproductive Toxicity
10143-60-9	di-2-Ethylhexyl ether	X ¹				
109-21-7	Butyl butyrate	X ²	X ³	X/X ³	X ³	X ³
126-30-7	Neopentyl glycol	X	X	X/X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X/X	X	X
71-36-3	n-butyl alcohol	X	X	X/X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X ⁴	X ^{5,6}	X/X ⁷	X ⁸	X ^{5,6}
NA	Alkyl Acetals					
104-76-7	2-Ethylhexanol	X	X	X/X	X	X
78-83-1	Isobutyl alcohol	X	X	X/X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X/X	X	X
107-92-6	Butyric acid	X	X	X/X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs.

1. Smyth, H.F. (1954). Range-Finding Toxicity Data: List V. *AMA Arch. Ind. Hyg. Occup. Med.* **10**, 61-68.
2. Butyl n-butyrate: Fragrance raw materials monographs. *Food Cosmetics Toxicology* **17**, 521-522 (1979); RTECS Number: ES8120000
3. Endpoint evaluated through use of surrogates butyric acid and n-butanol
4. Ballantyne, B. (1985). The Acute Toxicity and Primary Irritancy of 2-Ethyl-1,3-Hexanediol. *Vet. Hum. Toxicol.* **27(6)**, 491-495.
5. VanMiller, J.P., et al. (1995). Repeated Exposure Toxicity of 2-Ethyl-1,3-Hexanediol by Cutaneous Applications to the Rat for 9 and 90 Days. *Vet. Hum. Toxicol.* **37(1)**, 33-36.
6. Stenback, F. and Shubik, P. (1974). Lack of Carcinogenicity of Some Commonly Used Cutaneous Agents. *Toxicol. Appl. Pharmacol.*, **30**, 7-13.
7. Slesinski, R.S., et al., (1988). In Vitro and In Vivo Evaluation of the Genotoxic Potential of 2-Ethyl-1,3-Hexanediol. *Toxicology*, **53(2-3)**, 179-198.
8. Neeper-Bradley, T.L., et al. (1994). Evaluation of the Developmental Toxicity Potential of 2-Ethyl-1,3-Hexanediol in the Rat by Cutaneous Application. *J. Toxicol. – Cut. & Ocular Toxicol.*, **13(3)**, 203-214.