SUMMARY OF DATA FOR CHEMICAL SELECTION

PROPARGYL ALCOHOL

CAS No. 107-19-7

BASIS OF NOMINATION TO THE CSWG

The nomination of propargyl alcohol to the CSWG is based on high production volume, exposure potential, and suspicion of potential carcinogenicity. Dr. Elizabeth Weisburger, a member of the American Conference of Governmental Industrial Hygienists (ACGIH) TLV Committee as well as the Chemical Selection Working Group (CSWG), provided a list of 281 chemical substances with ACGIH recommended TLVs for which there were no long-term studies cited in the supporting data and no designations with respect to carcinogenicity. She presented the list to the Chemical Selection Planning Group (CSPG) for evaluation as chemicals which may warrant chronic testing; it was affirmed at the CSPG meeting held on August 9, 1994, that the 281 "TLV Chemicals" be reviewed as a Class Study. As a result of the class study review, propargyl alcohol is presented as a candidate for testing by the National Toxicology Program because of:

- potential for occupational exposures based on moderately high production volume
- evidence of occupational exposures based on TLV and other literature documentation
- potential for human exposures based on hazardous waste occurrences in environmental media
- suspicion of carcinogenicity based on mixed results in available short-term assays for genetic toxicity and liver and kidney changes in subchronic mammalian toxicity studies
- lack of chronic toxicity data.

Sources of human exposure to propargyl alcohol are mainly occupational; and the exposure potential is considered moderate based on an estimated U.S. annual production volume range of 0.5 to 2.8 million pounds, an estimate of 54,358 worker exposures (19,933 female) reported in the NOES database, and characterization of propargyl alcohol as a moderately volatile liquid identified in air, water, and soil.

Genetic toxicity test results include a negative Ames/*Salmonella* assay, weak mutagenic activity without metabolic activation in *S. typhimurium* strain D3052, positive for chromosomal

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aberrations in Chinese hamster ovary cells both with and without activation, and a negative result in a mouse micronucleus assay. Liver and kidney changes, including degenerative damage, were seen in subchronic inhalation and oral studies in rats. Metabolism to the more mutagenic aldehyde, 2-propyn-1-al, has been observed in mammalian systems.

SELECTION STATUS

ACTION BY CSWG: 12/6/95

Studies Requested: Subchronic studies

Priority: Moderate

Rationale/Remarks:

- High production volume
- Potential for human exposure
- Suspicion of carcinogenicity based on metabolism to the aldehyde and some positive results in some genotoxicity studies (Chinese hamster ovary cells, and *Salmonella*
- Hepatotoxicity observed in previous studies is similar to that produced by carbon tetrachloride

INPUT FROM GOVERNMENT AGENCIES/INDUSTRY

Dr. John Walker, Executive Director of the TSCA Interagency Testing Committee, was contacted at EPA for information on the total annual production level of propargyl alcohol. Dr. Walker reported it to be within a range of 0.5 to 2.8 million pounds for 1989 (Walker, 1995a). He also provided a summary of actions of the TSCA ITC on this chemical (see Regulatory Status section).

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CHEMICAL IDENTIFICATION

CAS Registry Number:	107-19-7
Chemical Abstract Name:	2-Propyn-1-ol (8CI, 9CI)
Synonyms:	Propargyl alcohol; propynyl alcohol; 2-propynol; 2-propynyl alcohol; 1-hydroxy-2-propyne; 1-propyn-3-ol; 1-propyn-3-yl alcohol; 3-hydroxy-1-propyne; 3-propynol; ethynylcarbinol; PA
Structural Class:	Alkynol (acetylenic alcohol)

Structure, Molecular Formula and Molecular Weight:

C_3H_4O Mol. wt.: 56.06

Chemical and Physical Properties

Description:	Light to straw-colored, moderately volatile liquid with geranium-like odor (ACGIH, 1993; STN International, 1995a)
Boiling Point:	114°C (ACGIH, 1993)
Melting Point:	-52°C (ACGIH, 1993)
Specific Gravity:	0.972 (Lington & Bevan, 1994)
Solubility:	Soluble in water, ethanol, benzene, acetone, chloroform and ether; insoluble in aliphatic hydrocarbons (ACGIH, 1993); forms azeotrophic mixture with water [BP, 97.5%] (Budavari, 1989)
Vapor Pressure:	11.6 mm Hg @ 20°C (Lington & Bevan, 1994)
Flash Point:	36°C, open cup (ACGIH, 1993)
Log P:	-0.38 (Sangster, 1989)

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Reactivity:	Flammable liquid; moderate fire risk (Sittig, 1985; Lewis, 1993); forms explosive peroxides (Eastman Fine Chemicals, 1990)

Technical Products and Impurities: According to Lewis (1993) propargyl alcohol is typically supplied in technical grade or in a 75% solution. It is available from catalog suppliers, Aldrich, Eastman Chemicals, and Janssen Chimica with a purity of 99% (Aldrich Chemical Co., Inc., 1994; Eastman Fine Chemicals, 1990; Janssen Chimica, 1992). Chem Service supplies it in Standard Grade both as a solid and in solution [100 μg/ml in methanol] (Chem Service, Inc., 1994).

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EXPOSURE INFORMATION

Production and Producers: Propargyl alcohol can be prepared from acetylene by high-pressure synthesis (Lewis, 1993). It is also captured as a by-product of the commercial synthesis of butynediol in several processes, typically with a yield of about 5% (Lington & Bevan, 1994). A patent has recently been assigned to GAF-Huels Chemie G.m.b.H. for high yield manufacture of propargyl alcohol from acetylene and formaldehyde by a single-step addition reaction with copper acetylide as catalyst and dimethoxymethane as solvent (Westernacher *et al.*, 1989). GAF-Huels has also been assigned a series of patents for the manufacture of propargyl alcohol by cleavage in varying solvent conditions of 2-butyn-1,4-diol in the presence of acetylene with copper acetylide as catalyst and elevated temperature and pressure (STN International, 1995b).

Propargyl alcohol is listed in the EPA's TSCA Inventory (STN International, 1995c). According to Lington and Bevan (1994) propargyl alcohol is the major commercially available acetylenic primary alcohol. The annual U.S. production of propargyl alcohol was reported to be in the range of 480,000-2,770,000 pounds based on non-confidential data received by the EPA for 1989 (Walker, 1995). No other quantitative information on annual production was found in the available literature. Propargyl alcohol is listed as a chemical in commerce in the U.S. International Trade Commission (USITC) publication, *Synthetic Organic Chemicals, US Production and Sales, 1990-1992* (USITC, 1991, 1993, 1994). The reporting company for each year was listed as ISP Chemicals, Inc., a Division of GAF Corp.; but no production or sales quantities were included. According to the USITC, separate statistics were not published to avoid disclosure of individual company operations. Although no specific production data were reported, the USITC reporting guidelines specify that each company's report of a chemical represents manufacturer of a quantity ≥ 4,500 kg [10,000 lbs] or sales ≥ $10,000. Based on a search of recent literature sources, including chemical industry catalogs, directories, and databases, the companies presented in Table 1 have been identified as producers/suppliers of propargyl alcohol, recent patent assignees for its preparation and/or use, or companies providing toxicity study results to the EPA in response to § TSCA 8(d) or 8(e) rules (Hunter, 1994; Kuney, 1994; Van, 1994; CIS, 1995; Krewson, 1995; STN International, 1995c, 1995d).

Imports: The following quantities of propargyl alcohol were reported to have been imported from points of origin in Europe to various U.S. ports and company destinations (importing

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companies not identified): > 60,000 lbs between January and August, 1995; > 171,000 lbs between March and December, 1994 (Dialog Information Services, 1995).

Use Pattern: Propargyl alcohol has several major use areas. They include: reactant/chemical intermediate; pharmaceutical intermediate; agricultural chemical intermediate; corrosion inhibitor; solvent stabilizer; and polymer modifier (ACGIH, 1992; Kuney, 1994; Lewis, 1993; STN International, 1995b). Some examples of these uses and some specialty or potential new uses are presented in Table 2.

In addition to the above uses, ACGIH (1993) and Lewis (1993) list "soil fumigant" as a use for propargyl alcohol. However, further literature and database searching failed to substantiate this use; and, responding to a request for information, Dr. Bill Burnham of EPA's Office of Pesticide Programs (OPP) reported that he was unable to locate any record of this chemical being used as a fumigant (Burnham, 1995).

Human Exposure: There is potential for human exposure to propargyl alcohol in occupational settings. According to Lington and Bevan (1994) propargyl alcohol is a moderately volatile liquid, and the primary routes of occupational exposure are inhalation and dermal contact. Verschueren (1983) reported an odor threshold concentration for propargyl alcohol of 0.35 mg/m^3.

The National Occupational Exposure Survey (NOES), which was conducted by the National Institute for Occupational Safety and Health (NIOSH) between 1981 and 1983, estimated that 54,358 workers, including 19,933 female employees, were potentially exposed to propargyl alcohol in the workplace. The NOES database does not contain information on frequency, level, or duration of exposure to workers of any chemicals listed therein (NIOSH, 1990)

Environmental Occurrence: Propargyl alcohol is not known to occur naturally. It has been identified as a pollutant in air, soil, and solid waste. In a study to assess relative incinerability rankings for 320 principal organic hazardous constituents (POHC), Taylor and coworkers (1990) listed propargyl alcohol in the first of three stability families, i.e., one of the 77 most stable and likely to be characterized by bimolecular decomposition processes.

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Table 1. Companies producing or supplying propargyl alcohol

	Producer/supplier listed in chemical industry catalog and/or directory	Company assigned patent for preparation and/or use	Company providing toxicity study data to EPA
Aceto Chemical Co./Pfaltz & Bauer	X		
Div.	X		
Aldrich Chemical Co., Inc.	X		
Alfa/Aesar Johnson Matthey	X		
Atomergic Chemetals Corp.		X	
Avon Products, Inc.	X		
BASF Corporation		X	
Chemlink, Inc.	X		
Chem Service, Inc.	X		
Crescent Chemical Co., Inc.		X	X
Dow Chemical Co.			X
Eastman Chemical Co./Eastman			X
Kodak	X		
Exxon Chemical Co.	X		
Fisher Scientific Co.	X	X	X
Fluka Chemical Corp.			
GAF Corp./International Specialty	X		
Products (ISP) Co.	X		
ICN Biomedicals, Inc.	X		
International Chemical Group			
Janssen Chimica/Spectrum Chemical	X		
Manufacturing Corp.		X	
Lancaster Synthesis, Inc.	X		
Nalco Chemical Co.	X		
Narchem Corp.			X
Penta Manufacturing		X	
Petrolite Corp.		X	
PPG Industries, Inc.	X		
Schering Corp.	X		
Supelco Inc.		X	
T.C.I. America, Inc.	X		
Upjohn Co.			
Wiley Organics, Inc.			

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Table 2. Uses of propargyl alcohol

Major Use Areas

Steel production chemical

- for prevention of hydrogen embrittlement of steel (ACGIH, 1992; Lewis, 1993)

Corrosion inhibitor

- component of solder fluxes (Minahara & Ikuta, 1992)
- component of scale-removing pickling agent (Matsuda *et al*., 1990; Kutej *et al*., 1993)
- for use in petroleum wells (Teeters, 1992)

Starting material/chemical intermediate

- pharmaceutical raw material (Krewson, 1995)
- starting material in synthesis of phospholipids for use as intermediates in preparation of macrocyclic diyne liposomes (Ladika *et al*., 1994)
- in electronics industry for synthesis of liquid crystals (Okabe *et al*., 1992)
- agricultural chemical intermediate (Kuney, 1994)

Stabilizer

- solvent stabilizer (ACGIH, 1992; Lewis, 1993)
- component/solvent in paints and coatings and in paint strippers for the aerospace industry (Anon., 1995; Sim, 1995)
- in electroless plating baths (Nakazawa *et al*., 1992)

Monomer/polymer starting material

- starting material for polydiacetylene-polyesters (Fomine *et al*., 1995)
- starting material for polysiloxane rubbers and sealants (Trego, 1989)
- monomer for synthetic fibers for electric conductors (Naarmann, 1994)
- monomer for adhesives and coating resins (Takiyama *et al*., 1989)

Other use areas

Miscellaneous/specialty uses

- laboratory reagent (Lewis, 1993)
- solvent for hydrochloric acid (Clever, 1989)
- gasoline additive to promote flame propagation in internal combustion engines (Takizawa *et al*., 1993)
- starting material in manufacture of brominated fire-proofing agents (Anon., 1975)

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Regulatory Status: The ACGIH-recommended threshold limit value-time weighted average (TLV-TWA) for propargyl alcohol is 1 ppm (2.3 mg/m^3) (ACGIH, 1992). The OSHA permissible exposure limit (PEL) is 1 ppm (2.3 mg/m^3) over an eight-hour work shift with a skin notation (ACGIH, 1992).

The Interagency Testing Committee (ITC) in its 28th Report recommended propargyl alcohol, without designating, for the acquisition of physical and chemical property data and biodegradation screening. The EPA has received several reports of unpublished health and safety data under a TSCA § 8(d) Health and Safety Data Reporting Final Rule (STN International, 1995b). Propargyl alcohol is classified as RCRA hazardous waste #P102 and is designated under EPA's CERCLA as a hazardous substance with a final rule for an adjusted reportable quantity (RQ) of 1,000 lbs (Environmental Protection Agency, 1989). In addition to identifying and listing propargyl alcohol as a hazardous waste, the EPA has set standards for treatment technologies appropriate to land disposal of wastewater and nonwastewater wastes containing propargyl alcohol (Environmental Protection Agency, 1991). This chemical has been added to the Toxic Release Inventory (TRI) and is, therefore, reportable under § 313 of the Emergency Planning and Community Right-to-Know Act (EPCRA) of 1986 and § 6607 of the Pollution Prevention Act of 1990 (Anon., 1995; STN International, 1995c).

The following is a summary of actions taken by the TSCA Interagency Testing Committee (ITC) on propargyl alcohol (Walker 1995b).

- Propargyl alcohol was added to the *Priority Testing List* in the 28th Report
- It was recommended for physical and chemical properties and biodegradation rate screening testing as part of a substructure-based class study (alkynes).
- It was removed from the Priority Testing List in the 32nd Report, before TSCA section 8(a) and 8(d) rules were published, because member agencies did not identify data needs and there were competing priorities.

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EVIDENCE FOR POSSIBLE CARCINOGENIC ACTIVITY

Human Data: No epidemiological studies or case reports investigating the association of exposure to propargyl alcohol and cancer risk in humans were identified in the available literature. No adverse effects in humans have been reported (Lington & Bevan, 1994).

Animal Data: No 2-year carcinogenicity studies of propargyl alcohol in animals were identified in the available literature. Toxicity information identified was limited to acute and subchronic studies which are summarized in Tables 3 and 4. Propargyl alcohol has a high order of acute toxicity by the oral, dermal, and inhalation routes of exposure. It is irritating to the eyes, skin, and respiratory tract. Repeated oral or inhalation exposure has produced liver and kidney damage in rats (Lington & Bevan, 1994). Following inhalation of propargyl alcohol, male and female rats exhibited fatty changes in the liver similar to those induced by carbon tetrachloride (Dow Chemical Co., 1964).

Table 3. Acute toxicity data for propargyl alcohol.

Route	Species/strain	Endpoint	Value	Reference
oral	rat(male)	LD_{50}	93 mg/kg	Vernot *et al*., 1977
oral	rat(male)	LD_{50}	110 mg/kg	Archer, 1985
oral	rat(female)	LD_{50}	54 mg/kg	Vernot *et al*., 1977
oral	rat(female)	LD_{50}	55 mg/kg	Archer, 1985
oral	mouse	LD_{50}	50 mg/kg	Rowe *et al*., 1982
oral	guinea pig	LD_{50}	60 mg/kg	Rowe *et al*., 1982
dermal	rabbit	LD_{50}	88 mg/kg	Vernot *et al*., 1977
dermal	rabbit	LD_{50}	16 mg/kg	Rowe *et al*., 1982
inhalation/1-hr	rat(male)	LC_{50}	1200 ppm	Vernot *et al*., 1977
inhalation/1-hr	rat(female)	LC_{50}	1040 ppm	Vernot *et al*., 1977

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Table 4. Subchronic toxicity data for propargyl alcohol

Route/Species	Dose/Duration	Result/Observations	Reference
dermal/rabbit	1, 3 or 10 mg/kg/day 5 days/week for 90 days (10 mg dose increased to 20 mg on day 63)	no systemic effects noted	GAF, 1965
preliminary inhalation/rat, mouse, guinea pig, rabbit, cat	100 ppm for up to 75 days	irritation of mucous membranes	BASF unpublished data [cited in Lington & Bevan, 1994]
inhalation/rat	80 ppm for 7 hr/day, 5 days/wk for 59 days during 89 day period	*gross*: increased liver weights/male; increased liver & kidney weights/female *histopath*: degenerative damage in kidneys and liver (more marked in female); fatty changes in liver similar to those induced by carbon tetrachloride	Dow Chemical Co., 1964
oral gavage/rat	0, 5, 15 or 50 mg/kg day for up to 92 days	*gross*: hematologic changes & enzyme changes characteristic of liver damage and increased liver & kidney weights at mid and high doses; *histopath*: kidney (karyomegaly of renal tubular epithelial cells) & liver (megalocytosis & cytoplasmic vacuolation) lesions at mid and high doses.	Rubenstein *et al*., 1989; Lington & Bevan, 1994

Short-Term Tests: Propargyl alcohol was not mutagenic in *Salmonella typhimurium* strains TA97, TA98, TA100, and TA102 when tested at doses up to 0.75 µl/plate with and without metabolic activation. To avoid artifactual results due to test chemical-solvent interactions, it was tested using 2 solvents, DMSO and water (Blakey *et al.*, 1994). Propargyl alcohol was also inactive in *S. typhimurium* strains TA1535, TA1537, and TA1538 both with and without activation (dose not reported) (Lington & Bevan, 1994). Without activation propargyl alcohol was a weak mutagen (15 revertants/µmol) in *S. typhimurium* strain D3052, a strain with intact excision repair but without plasmid pKM101 that codes for the error-prone repair enzyme of the SOS system. The specific mutagenicity did not increase in the presence of a metabolic activation system (Basu & Marnett, 1984).

In Chinese hamster ovary (CHO) cells collected 16 hours following treatment, propargyl

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alcohol, administered in 0, 2.0, 3.0, 6.0, and 10 mM doses without metabolic activation, induced a statistically significant increase ($P < 0.05$) in chromosomal aberrations (CA) at the highest dose. When doses of 0, 0.4, 0.6, 0.8, and 1.0 mM were administered with activation, a larger dose-related increase ($P \leq 0.001$) was induced. In cells sampled 10 hours following propargyl alcohol treatment, there were no increases in aberrations (Blakey *et al.*, 1994)

Propargyl alcohol did not induce micronuclei *in vivo* in the mouse bone-marrow micronucleus assay following administration of doses of 24, 28, or 72 mg/kg by gavage to male and female mice (Blakey *et al.*, 1994).

Metabolism: According to Williams (1959) primary aliphatic alcohols undergo two general types of metabolic reactions, oxidation to carboxylic acids and direct conjugation with glucuronic acid. He further stated that the extent of glucuronidation depends on the speed of the oxidation reaction, but no information was reported specifically on alkynols or propargyl alcohol. DeMaster and coworkers (1994) reported that, while oxidative metabolism of low molecular weight saturated and unsaturated primary alcohols is generally accepted to be catalyzed by alcohol dehydrogenase, propargyl alcohol is a relatively poor substrate for this enzyme. In their study of the metabolism of propargyl alcohol by an alternative pathway utilizing bovine liver catalase, they measured the rate of oxidative bioactivation of propargyl alcohol to 2-propyn-l-al and found it to be higher than predicted according to a correlation analysis based on molecular size (volume) and to be 30% greater than the oxidative rate determined for ethanol. Furthermore, 2-propyn-l-al inhibited the peroxidative and catalytic activities of the catalase. Based on their findings, DeMaster and coworkers (1994) hypothesized that the oxidative biotransformation of propargyl alcohol to the more reactive α,β-unsaturated aldehyde by liver catalase might be the initial step in propargyl alcohol-induced liver injury; and they stated a need for additional study to elucidate the role of alternative oxidative pathways in this process including oxidation by hydroxyl radicals and the microsomal cytochrome P450-catalyzed reaction.

Intraperitoneal (ip) administration of 1.25 mmol/kg propargyl alcohol followed by ethanol to Sprague Dawley rats led to more than 80% inhibition of hepatic mitochondrial aldehyde dehydrogenase (AIDH) and caused a rise in blood acetaldehyde (AcH) quantitatively similar to that from the drug pargyline. Propiolaldehyde (2-propyn-l-al), a metabolic product common to both propargyl alcohol and pargyline, was identified as the major metabolite responsible

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for the *in vivo* inhibition of AIDH (DeMaster *et al.*, 1986). Pargyline did not inhibit rat mitochondrial AIDH *in vitro.* However, with 200 µM propargyl alcohol or 200 µM propiolaldehyde inhibition was 19% and 96%, respectively (DeMaster & Nagasawa, 1978).

Basu and Marnett (1984) noted that the mutagenicity of propargyl alcohol in *S. typhimurium* D3052 was probably due to its partial oxidation to propynal by bacterial enzymes.

Structure/Activity Relationships: Six compounds, structurally similar to propargyl alcohol, were screened for relevant information associating these related chemicals with a mutagenic or carcinogenic effect. A summary of information found in the available literature is presented in Table 5 followed by a more detailed discussion. No information was found on carcinogenicity or mutagenicity for three of these structurally related compounds; butynol [11069-20-8], 2-butynol [764-01-2], and 3-butynol [927-74-2]. Information on carcinogenicity was identified for only one of the compounds, allyl alcohol. The significance of exposure to allyl alcohol and the incidence of lymphatic and hematopoietic tissue cancer in a chemical manufacturing environment was confounded by the multiple-chemical exposure of employees. Allyl alcohol was nontumorigenic in rat and hamster assays. Allyl alcohol caused no acceleration of hepatic nodules in SMA/MS mice fed 2,7-bis(acetamido)fluorene (2,7-AAF). Mutagenicity data were available for three of the structurally related compounds. Allyl alcohol was mutagenic in mouse lymphoma and Chinese hamster V-79 tests. Positive results were also reported in *S. typhimurium* strains TA100 and TA1535. Allyl alcohol was not mutagenic in *Streptomyces coelicolor* or *Aspergillus nidulans.* 2-Propynal was mutagenic in *S. typhimurium* strain D3052 while propiolic acid was negative in this strain; both compounds were negative in strains TA98 and TA100.

Carcinogenic Effects

Allyl alcohol. Nested case-control studies of non-Hodgkin's lymphoma, multiple myeloma, nonlymphocytic leukemia, and lymphocytic leukemia were conducted within a cohort of employed men from three Union Carbide facilities. Exposure odds ratios were examined in relation to 111 work areas, 21 specific chemicals (including allyl alcohol), and 52 chemical activity groups. The exposure odds ratios by ever/never classification of having worked with allyl alcohol for each disease were as follows; non-Hodgkins lymphoma 2.6 (2 cases); multiple myeloma 2.6 (1 case), nonlymphocytic leukemia 2.5 (1 case), and lymphocytic leukemia (no cases). The significance of findings for individual chemicals was confounded by the multiple-

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chemical exposure of employees (Ott *et al.*, 1989a,b).

Lijinsky and Reuber (1987) examined the carcinogenic effects of chronic exposure to allyl alcohol in rats and hamsters. Groups of 20 male and female F344 rats were given 300 mg/l allyl alcohol in drinking water 5 days a week for 2 years. Twenty male Syrian hamsters were administered 2 mg allyl alcohol by gavage once a week for 60 weeks. There were no statistically significant increases in incidences of neoplasms in rats or hamsters related to allyl alcohol administration. Allyl alcohol treatment caused no apparent acceleration in the induction of hepatic nodules in groups of 10 to 16 male and female SMA/Ms mice fed 2,7-AAF. Male mice were given 5 ml of 1% allyl alcohol/kg body weight in aqueous solution by gavage once a week for 8 weeks administered concurrently with 0.025% 2,7-AAF in the diet. Female mice received 8 gavage treatments of allyl alcohol administered alternately with 2,7-AAF in the diet 1 week a month for 32 weeks (Kozuka & Sassa, 1976).

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Table 5. Summary of Information on Propargyl Alcohol and Structurally Related Compounds

Chemical name [CAS RN]	Carcinogenicity data	Mutagenicity data
Propargyl alcohol [107-19-7] $HC{\equiv}CCH_2OH$	NDF	negative in *S. typhimurium* TA97, TA98, TA100, TA102, TA1535, TA1537, and TA1538 with and without activation (Blakey *et al.*, 1994; Lington & Bevan, 1994) weak positive in *S. typhimurium* D3052 without activation (Basu & Marnett, 1984) positive for CA in CHO cells with and without activation (Blakey *et al.*, 1994) negative in mouse bone marrow micronucleus assay (Blakey *et al.*, 1994)
Allyl alcohol [107-18-6] $H_2C{=}CHCH_2OH$	significance of exposure to allyl alcohol and occurrence of lymphatic and hematopoietic tissue cancer in a chemical manufacturing environment not determined (Ott *et al*., 1989a,b) nontumorigenic in male and female F344 rats in 2-year oral bioassay (Lijinsky & Reuber, 1987) nontumorigenic in male Syrian hamsters in 60-week gavage study (Lijinsky & Reuber, 1987) no acceleration of 2,7-AAF-induced hepatic nodules in male or female SMA/MS mice (Kozuka & Sassa, 1976) subchronic tests on rats and mice in progress (NTP, 1995a)	negative in *S. typhimurium* TA1535, TA1537, TA1538, TA98, TA100 with and without activation (spot test); negative TA1535, TA100, TA98 with and without activation (plate test) (Principe *et al.*, 1981) negative in *S. typhimurium* TA1537, TA1538, TA98, TA100 with and without activation (preincubation and plate tests) (Lijinsky & Andrews, 1980) positive in *S. typhimurium* TA100 without activation, weak mutagenicity with activation (liquid suspension test) (Lutz *et al.*, 1982) positive in *S. typhimurium* TA1535 with hamster S-9 (preincubation test) (Lijinsky & Andrews, 1980) negative in *S. typhimurium* and mouse lymphoma assays (NTP, 1995b) positive mouse lymphoma L5178Y without activation (NLM, 1995) positive in V79 cells for 6-thioguanine resistance (Smith *et al.*, 1990) negative in *S. coelicolor* and *A. nidulans* (Principe *et al.*, 1981)
2-Propynal [624-67-9] $HC{\equiv}CC(O)H$	NDF	positive in *S. typhimurium* D3052 without activation, negative in TA98, TA100 (Basu & Marnett, 1984)
Propiolic acid [471-25-0] $HC{\equiv}CCO_2H$	NDF	negative in *S. typhimurium* D3052, TA98, TA100 (Basu & Marnett, 1984)

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Mutagenic Effects

Allyl alcohol. The mutagenicity of allyl alcohol has been tested in the DCB Short-term Test Program of the National Cancer Institute. Positive results were obtained in the mouse lymphoma assay when allyl alcohol was tested at 1.5-9.2 µl/ml without metabolic activation (NLM, 1995). Allyl alcohol was tested in *S. typhimurium* strains TA98, TA100, TA1535, TA1537, and TA1538 using a variety of treatments (standard plate or preincubation) and solvents (water or DMSO). Positive results were reported only in TA1535 at 10-500 µg/plate using the preincubation method with water as the solvent and hamster liver S9 activation (Lijinsky & Andrews, 1980). Lutz and coworkers (1982) reported positive results when allyl alcohol was tested in TA100 using the preincubation method and DMSO as the solvent. Revertants per µmole were 750 without activation and 145 with S9. Principe and coworkers (1981) tested the mutagenicity of allyl alcohol in *S. typhimurium* strains TA98, TA100, TA1535, TA1537, and TA1538 as well as in *Streptomyces coelicolor* and *Aspergillus nidulans*. Allyl alcohol was negative in all test systems. At 1 and 2 µM doses, allyl alcohol was mutagenic in V-79 cells using 6-thioguanine resistance as the measure of mutagenicity (Smith *et al.*, 1990).

2-Propynal. Propynal induced 1370 revertants/µmol in *S. typhimurium* strain D3052. Results were negative with strains TA98 and TA100 (details not reported) (Basu & Marnett, 1984). The authors postulated a mechanism whereby this compound exhibits mutagenicity following nucleophilic addition resulting in a substituted acrolein.

Propiolic acid. Propiolic acid was not mutagenic in *S. typhimurium* strains D3052, TA98 and TA100 (details not reported) (Basu & Marnett, 1984).

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