Chemical Information Profile

for

Dimethylamine Borane
[CAS No. 74-94-2]

Supporting Nomination for Toxicological Evaluation by the National Toxicology Program

July 2008

National Toxicology Program
National Institute of Environmental Health Sciences
National Institutes of Health
U.S. Department of Health and Human Services
Research Triangle Park, NC
http://ntp.niehs.nih.gov/

Data Availability Checklist for Dimethylamine Borane [74-94-2]

Abbreviations: H = human; L = *Lepus* (rabbit); M = mouse; R = rat
Note: No judgement of whether the available data are adequate for evaluation of these endpoints in the context of human health hazard or risk assessment has been made.

ENDPOINT	H	M	R	L	ENDPOINT	H	M	R	L
ADME					**Developmental Toxicity**				
Absorption					Developmental abnormalities				
Distribution					Embryonic/fetal effects				
Metabolism					Newborn effects				
Excretion					**Carcinogenicity**				
Acute Toxicity (up to 1 week)					Dermal				
Dermal	X		X		Inhalation				
Inhalation					Oral				
Injection		X	X	X	**Anticarcinogenicity**				
Ocular					Anticarcinogenic effects				
Oral	X	X	X		**Genotoxicity**				
Subchronic Toxicity (1 to <26 weeks)					Cytogenetic effects				
Dermal					Microbial gene mutation				
Inhalation					Gene mutation *in vitro*				
Injection					Gene mutation *in vivo*				
Oral					Germ cell effects				
Chronic Toxicity (≥26 weeks)					**Neurotoxicity**				
Dermal					Behavioral activity	X			
Inhalation					Motor activity	X			
Injection					**Immunotoxicity**				
Oral					Immunotoxic effects				
Synergism/Antagonism					**Cardiovascular Toxicity**				
Synergistic effects					Cardiovascular effects				
Antagonistic effects					**Mechanistic Data**				
Cytotoxicity					Target Organs/Tissues				
Cytotoxic effects					Endocrine modulation				
Reproductive Toxicity					Effect on enzymes				
Fertility effects					Modes of action	X			
Maternal effects					Effect on metabolic pathways				
Paternal effects					**Structure-Activity Relationships**	X	X	X	X

The above table provides an overview of the data summarized in the profile by endpoint and species. The endpoints are listed in columns 1 and 6 and the species (human, rat, mouse, and rabbit) are represented by columns 2-5 and 7-10. An "**X**" is displayed in each box corresponding to an endpoint (row) and species (column) for which data are reviewed. An empty box indicates that data for the corresponding endpoint and species were not available.

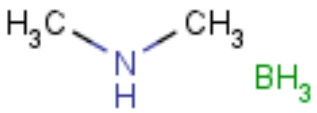
Dimethylamine Borane Nomination Summary

Chemical Name: Dimethylamine borane

CAS RN: 74-94-2

Formula: $C_2H_{10}BN$

Molecular Wt.: 55.89



Basis for Nomination: Dimethylamine borane (DMAB) was nominated by the assistant-coordinator of the National Institute of Occupational Safety and Health (NIOSH) Dermatology Cross-Sector (National Occupational Research Agenda's Immune and Dermal Diseases Cross-Sector Council) for dermal absorption, dermal toxicity, and skin sensitization studies. DMAB was identified as a possible contact sensitizer and systemic toxicant and is being considered for inclusion into the NIOSH Chemical Pocket Guide. A review of the dermatology literature by the Dermal Subject Matter Expert Workgroup for evidence of adverse effects failed to provide sufficient scientific evidence for the group to make a recommendation.

DMAB is produced by the reaction of diborane with dimethylamine or a borohydride with an amine (e.g., dimethylamine, dimethylammonium salt, or amine hydrochloride salt). From 1994-2002, production volumes (reported under the Inventory Update Rule) ranged between 10,000 and 500,000 pounds. DMAB is used in a variety of reactions to reduce chemicals in organic and inorganic chemistry, such as aldehydes and ketones to alcohols. It also serves as a reducing agent in electrolysis deposition of metals, alloys, semiconductors, and insulators.

DMAB is reported to cause irritation in the eyes, skin, and respiratory tract. In one case study, four workers accidentally exposed either dermally or orally to a formulation containing 97% DMAB experienced dizziness, nausea, vomiting, and gastrointestinal issues. Three workers were immediately decontaminated and endured no additional side effects, while the individual who did not shower until >1 hour later experienced long lasting neurological impairment (acute cerebral and cerebellar alterations and peripheral neuropathy). DMAB is also an irritant in rabbit eyes and skin; a dermal LD_{50} of 210 mg/kg was reported. Additionally, an oral LD_{50} of 59 mg/kg has been calculated for the rat, and intraperitoneal LD_{50} values of 40, 200, 35, and 56 mg/kg have been given for the rat, mouse, rabbit, and guinea pig, respectively. DMAB was active in the National Cancer Institute *in vivo* anticancer drug screen for tumor model L1210 leukemia in BDF1 mice. No other toxicological information was available.

A. Chemical Information

Molecular Identification

Chemical Name: Dimethylamine borane (DMAB)
CAS RN: 74-94-2
Synonyms: Dimethylamine borane (1:1); EINECS 200-823-7; NSC 10218; Dimethylamine compound with borane (1:1); Borane, compd. with dimethylamine (1:1); Dimethylamine, compd. with BORANE (1:1); N-Methylmethanamine compd. with borane (1:1); Borane, compd. with N-methylmethanamine (1:1); Boron, (N-methylmethanamine)trihydro-, (T-4)-; Boron, trihydro(N-methylmethanamine)-, (T-4)-; Boron, trihydro(N-methylmethanamine)-, (beta-4)-; Methanamine, N-methyl-, compd. with borane (1:1) (9CI); Borane-dimethylamine complex; Borane-dimethylamine; Boron hydride-dimethylamine; Methanamine, N-methyl-, compd. with borane (1:1)
Trade Names: Lectroless® AU 2000 Unit B (<10% DMAB and <5% potassium hydroxide in water [w/w]); Enbond® Xtra (<10% DMAB and <5% sodium hydroxide in water [w/w]) (Enthone-OMI, 2002a,b)
Hill Formula: C2H10BN
Line Formula: $(CH_3)_2$-NH:BH_3
Smiles Notation: [B].CNC
PubChem CID: 6328035 (PubChem, undated)
InChI: 1/C2H7N.B/c1-3-2;/h3H,1-2H3
Molecular Weight: 55.8947
Purity of Commercial Products: ≥97% (BASF, 2005; Sigma-Aldrich, 2006, 2007)
Impurities in Commercial Products: Dimethylamine (BASF, 2005)
Biodegradation Products: Product has not been tested, but is proposed not to be biodegradable based on products of similar structure and composition (BASF, 2005)

Physical-Chemical Properties

Physical State: White to off-white crystalline solid (BASF, 2005; Sigma-Aldrich, 2006, 2007)
Specific Gravity or Density: Not available
Vapor Pressure: Not available
Solubility: 12.8% in other solvents (BASF, 2005)
Log P = Log K_{ow}: -0.51 @ 25 ºC (calculated) (BASF, 2005)
Bioconcentration Factor(s) (species): Not available

B. Exposure Potential

U.S. Annual Production

1986-1990: No reports
1994-2002: 10,000 – 500,000 pounds
(U.S. EPA, 2006a [U.S. EPA IUR database; search by casno = 74942])

Worldwide Annual Production

Not available

Production Processes

- Diborane and dimethylamine are reacted at a ratio of 1:2 at temperatures between ~0 and 50ºC. DMAB is removed as a liquid and allowed to crystallize at room temperature (Schechter et al., 1964 pat.).
- An electric current is passed between an inert anode and a cathode in a solution of a borohydride (e.g., sodium borohydride) and dimethylamine (Schechter et al., 1960 pat.).
- Reaction of an alkali metal or alkaline earth metal borohydride with a dimethylammonium salt. (Holzner et al., 1996 pat.).
- Reaction of amine hydrochloride salt with a borohydride (Lane, 2006).

- Reaction of amine with sodium borohydride under a variety of reaction conditions (e.g., with carbon dioxide in an inert solvent in the presence of water; in liquid sulfur dioxide; under anhydrous conditions with carbon dioxide) (Lane, 2006).

Uses

- Used in a variety of reactions to reduce chemicals in organic and inorganic chemistry (e.g., aldehydes and ketones to alcohols; Schiff bases to acetic acid; and quinones to hydroquinones) (Büchner and Niederprüm, 1977)
- Used as a reducing agent in electroless deposition of metals, alloys, semiconductors, and insulators (Liu et al., 2005)

Occupational Exposure

Not available

Exposure Limits (Standards and Criteria): Not available

General Population Exposure

Foods and Beverages, Cosmetics, etc.: Not available

Ambient Environment: Not available

Environmental Occurrence

Natural Occurrence: Boranes do not occur in nature. The smallest borane has the formula BH_3, which instantly dimerizes, therefore making the isolation of pure borane impossible. Instead, borane exists as the toxic gas diborane. When diborane is treated with an ether or amine, a stable complex is formed; this complex acts chemically like borane (Cotton and Wilkinson, 1962; Farlex, 2008).

U.S. Environmental Releases: Not available

Concentrations in Environmental Media: Not available

Regulatory Status

U.S. Environmental Protection Agency: Listed under TSCA Section 8(b) (Chemical Inventory Section) (U.S. EPA, 2006b)

Food and Drug Administration: Not available

C. Toxicological Information

Summary

DMAB causes eye, skin, and respiratory irritation and is toxic if swallowed. DMAB toxicity information includes acute toxicity in several species by different routes of exposure, DNA inhibition, and one case study of neurotoxicity from occupational exposure. Anti-tumor activity was also reported.

General Toxicity

Human Studies:

- DMAB causes eye, skin, and respiratory tract irritation. Additionally, sensitization may occur due to chemical contact with the skin. DMAB is toxic if swallowed (BASF, 2005).
- One case study and field investigation reported four workers had accidental exposure to a formulation containing DMAB (97% DMAB; 3% decomposition materials including boric acid, borates, hydrogen, and dimethylamine). Exposures were either dermal or oral. All individuals experienced dizziness, nausea, vomiting, and gastrointestinal issues. Three individuals were treated immediately after exposure (shower or water consumption) and had no additional side effects. The fourth individual decontaminated >1 hour after exposure and experienced long lasting neurological impairment (see ***Neurotoxicity*** section) (Tsan et al., 2005).

Animal Studies: Irritant in rabbit eye and skin studies (BASF, 2005; RTECS, 2006)

Chemical Disposition, Metabolism, and Toxicokinetics

Single citation available which discusses distribution and excretion of boranes (Levinskas et al., 1956)

Acute Exposures

LD_{Lo}/LD_{50} Values:

Oral:

LD_{50} = 59 mg/kg [rat] (ChemIDplus, undated)
LD_{Lo} = 50 mg/kg [mouse] (ChemIDplus, undated)
LD_{Lo} = 50 mg/kg [guinea pig] (ChemIDplus, undated)

Intraperitoneal (i.p.):

LD_{50} = 39 mg/kg [rat] (ChemIDplus, undated)
LD_{50} = 40 mg/kg [rat] (Levinskas, 1955)
LD_{50} = 200 mg/kg [mouse] (ChemIDplus, undated)
LD_{50} = 35.10 mg/kg [rabbit] (ChemIDplus, undated)
LD_{50} = 55.9 mg/kg [guinea pig] (ChemIDplus, undated)

Intravenous (i.v.):

LD_{50} = 56 mg/kg [mouse] (ChemIDplus, undated)

Dermal:

LD_{50} = 210 mg/kg [rabbit] (ChemIDplus, undated)

Subchronic Exposures

Not available

Chronic Exposures

Not available

Synergistic/Antagonistic Effects

Not available

Cytotoxicity

Not available

Reproductive and Developmental Toxicity

Not available

Carcinogenicity

Not available

Anticarcinogenicity

Human Studies: Not available

Animal Studies: Active in the NCI *in vivo* anticancer drug screen for tumor model L1210 leukemia in BDF1 mice (NCI, 2007)

Genetic Toxicity

Microbial Gene Mutation: Not available

Human Studies (*in vitro* and *in vivo*): Not available

Animal Studies (*in vitro* and *in vivo*): Not available

Germ Cell Effects: Not available

Neurotoxicity

Case study with a single individual that did not decontaminate from DMAB exposure for >1 hour showed long lasting neurotoxicological effects in the peripheral system. Acute cerebral and cerebellar alterations and peripheral neuropathy were observed. Alterations included decreased amplitudes of peripheral compound muscle action potentials (CMAP), prolonged distal latencies of CMAP, decreased nerve conduction velocities, and axonal degeneration (Kuo et al., 2006 ; Tsan et al., 2005).

Immunotoxicity

Not available

D. Mechanistic Data

Target Organs/Tissues

Not available

Endocrine Modulation

Not available

Effect on Enzymes

Not available

Modes of Action

Human: Toxic effects are potentially associated with decomposition products of DMAB (boric acid, hydrogen, borates, and dimethylamine). However, further studies are needed (BASF, 2005; Tsan et al., 2005). One older study suggests that toxicity of boranes correlates with reducing capacity (Hill et al., 1958).

Animal: Not available

Effect on Metabolic Pathways: Not available

Structure-Activity Relationships

Congeners/Metabolites:

- Dimethylamine [CAS No. 124-40-3; PubChem CID:674 (PubChem, undated)] could potentially be a metabolite of DMAB *in vivo*; however, no information was available to confirm this. According to the NIOSH National Occupational Exposure Survey (1981-1983), an estimated 28,879 workers (2001 females) are potentially exposed to dimethylamine in the United States (HSDB, 2008).

  ADME: Dimethylamine is a normal constituent in the stomach and urine of animals and humans. Human gastric fluid contains ~13 nmol/mL dimethylamine; saliva and blood contain similar amounts. The average urinary output in healthy volunteers was measured at ~17 mg/day. Dimethylamine is formed from trimethylamine via trimethylamine N-oxide and also probably from dietary lecithin and creatine; it is readily absorbed mostly from the small intestine and excreted in the urine (95% unchanged). When rats were orally administered a commercial diet containing DMA (23.6 ppm) or a low-DMA diet (1 ppm) for a week, excretion of DMA was 432.6 and 272.5 µg/animal, respectively, in the urine. In an inhalation study with rats, disposition of ^{14}C-dimethylamine at a low and high dose (10 and 175 ppm) was similar with >90% of the radioactivity in the urine and feces, 7-8% in various tissues, and 1.5% in exhaled $^{14}CO_2$ at 72 hours (HSDB, 2008).

  Acute Exposure: The following acute toxicity values have been reported:

  LD_{50}: oral (mg/kg) — 316 (mouse), 698 (rat), 240 (guinea pig, rabbit)
  i.p. (mg/kg) — 736 (mouse)
  dermal (mg/kg) — 3900 (rat)

  LC_{50}: ~14 mg/L (2 hr) (mouse); 2.3 mg/L (2 hr) to 8.8 mg/L (4 hr) (rat)

  Dimethylamine was sensitizing in a guinea pig maximization test, guinea pig closed epicutaneous test, and the ear swelling test in guinea pigs and mice. It is an eye, sensory, and respiratory irritant in mice. It caused damage in the rabbit eye (e.g., corneal edema) and skin (e.g., ulceration). Inhalation of dimethylamine (813-5420 ppm) produced ocular and respiratory irritation, cyanosis, convulsions, and death in mice; massive hemorrhages were observed near the periphery of the lungs and peripheral emphysema. In rats, effects ranging from ulceration and necrosis to rhinitis, tracheitis, and emphysema were observed (600-6000 ppm) (HSDB, 2008).

  Short-Term Exposure: Inhalation of dimethylamine (511 ppm 6 hr/day for 5 days) produced decreased body weight, nasal lesions, and death in mice. Dimethylamine (175 ppm 6 hr/day for 9 days) inhibited mucociliary function in rats. During a 90-day study, dimethylamine (5 ppm) produced no deaths or signs of toxicity in rats, guinea pigs, rabbits, dogs, and a monkey; histopathologically, interstitial inflammatory changes were observed in the lungs of all species. Inhalation of dimethylamine (97 or 183 ppm) for 18-20 weeks produced corneal injury in guinea pigs and rabbits and central lobular fatty degeneration and necrosis of parenchymal cells of the liver in mice, rats, guinea pigs, and rabbits. When added to the diet of rats for 3.5 months, dimethylamine (150 mg/kg) increased liver demethylase activity (HSDB, 2008).

Chronic Exposure/Carcinogenicity: In a TSCA Test Submission, inhalation of dimethylamine (10-175 ppm) for two years resulted in decreased relative kidney weights in rats given the low and mid doses, increased body weights in treated rats compared to controls at the mid dose, and decreased body weights and improved mortality compared to controls at the high dose. High-dose rats also had thinning nasal turbinates and increased phosphatase and serum glutamic oxaloacetic transaminase levels. Treated rats also had degenerative lesions in the respiratory and olfactory epithelia of the nasal cavity and an increased incidence of uterine stromal polyps. In a similar study using both rats and mice, dimethylamine produced decreased body weight and progressive inflammatory, degenerative, and hyperplastic lesions of the nasal passages of both species but no increase in tumor incidence. According to the American Conference of Governmental Industrial Hygienists, dimethylamine is "not classifiable as a human carcinogen" (A4 carcinogenicity rating) (HSDB, 2008).

Reproductive Toxicity: Inhalation of dimethylamine (183 ppm) for 18-20 weeks produced tubular degeneration of the testes in rabbits (HSDB, 2008).

Genotoxicity: Dimethylamine was negative for mutagenicity in *Salmonella typhimurium* strains TA98, TA100, TA1535, and TA1537 in the presence and absence of metabolic activation (S9) but positive in TA1530 with S9 using the standard plate method (CCRIS, 1993). It was also negative for forward and reverse gene mutation in the host-mediated assay (GENETOX, 1992). As a pyrolyzate, it was mutagenic in strains TA98 and TA100 with and without S9 (HSDB, 2008).

- Over 20 studies indicate that amine carboxyboranes and amine cyanoboranes have a variety of antineoplastic/cytotoxic, hypolipidemic, anti-inflammatory, anti-osteoporotic activities (e.g., Hall et al., 1994; Spielvogel et al., 1982 pat., 1994 pat.).
- See Appendix for information on DMAB analogs.

Reactive Moieties: Not available

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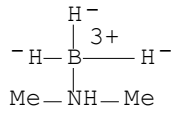
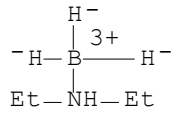
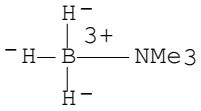
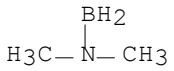
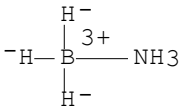
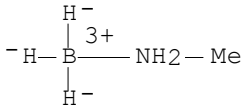
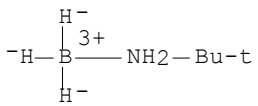
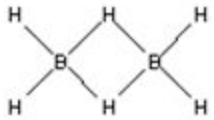
Appendix. SAR Information for Selected Analogs of Dimethylamine Borane [CAS No. 74-94-2] [1]

Chemical or Trade Name and Synonyms	CAS Registry Number®	Structure	Pharmacological Activities and Additional Comments
Boron, trihydro(N-methylmethanamine)-, (T-4)- Dimethylamine borane (1:1); EINECS 200-823-7; NSC 10218; Dimethylamine compound with borane (1:1); Borane, compd. with dimethylamine (1:1); Dimethylamine, compd. with BORANE (1:1); N-Methylmethanamine compd. with borane (1:1); Borane, compd. with N-methylmethanamine (1:1); Boron, (N-methylmethanamine)trihydro-, (T-4)-; Boron, trihydro(N-methylmethanamine)-, (T-4)-; Boron, trihydro(N-methylmethanamine)-, (beta-4)-; Methanamine, N-methyl-, compd. with borane (1:1) (9CI); Borane-dimethylamine complex; Borane-dimethylamine; Boron hydride-dimethylamine; Dmab; Methanamine, N-methyl-, compd. with borane (1:1)	74-94-2		The structure and synonyms for DMAB are included for comparison with analog structures and nomenclature.
Boron, (N-ethylethanamine)trihydro-, (T-4)- (9CI) Borane, compd. with N-ethylethanamine (1:1); Diethylamine, compd. with BH3 (6CI); Diethylamine, compd. with BH3 (1:1) (7CI); Diethylamine, compd. with borane (1:1) (8CI); Ethanamine, N-ethyl-, boron complex; Ethanamine, N-ethyl-, compd. with borane (1:1); (Diethylamine)trihydroboron; Diethylamine borane	2670-68-0		Not available

Chemical or Trade Name and Synonyms	CAS Registry Number®	Structure	Pharmacological Activities and Additional Comments
Boron, (N,N-dimethylmethanamine)trihydro-, (T-4)- Borane, compd. with N,N-dimethylmethanamine (1:1); Borane, compd. with trimethylamine (1:1) (8CI); Borine, compd. with Me3N (1:1) (6CI); Methanamine, N,N-dimethyl-, compd. with borane (1:1); Trimethylamine, compd. with borane (1:1) (8CI); Borane complex with trimethylamine (1:1); Borane-trimethylamine (1:1); NSC 10220; NSC 145941; NSC 53323; Trihydro(trimethylamine)boron; Trimethylamine borane(3); Trimethylamine-borane (1:1); Trimethylamineborane	75-22-9		**i.p. LD_{50} mouse** = 140 mg/kg (ChemIDplus, undated-a; Hall et al., 1985 [PMID:4032249]) **i.p. LD_{50} rat** = 175 mg/kg (ChemIDplus, undated-a) EPA TSCA: Section 8(b) [chemical inventory section] Inactive in NCI *In Vivo* Anticancer Drug Screen. Data for tumor model P388 and L1210 Leukemias (i.p.) in CD2F1 (CDF1) and B6D2F1 (BDF1) mice, respectively (PubChem, Undated [CID:6327651])
Boranamine, N,N-dimethyl- (9CI) Borane, (dimethylamino)- (7CI, 8CI); Borine, dimethylamino- (6CI); Boryldimethylamine; Dimethylaminoborane	1838-13-7		Not available
Boron, amminetrihydro-, (T-4)- (9CI) Borane, ammoniate (7CI); Borane, monoammoniate (8CI); Borine, ammoniate (6CI); Ammineborane; Amminetrihydroboron; Ammonia borane; Ammonia compd. with borane (1:1); Borazane	13774-81-7		Not available
Boron, trihydro(methanamine)-, (T-4)- (9CI) Borane, compd. with methanamine (1:1); Borane, compd. with methylamine (1:1) (8CI); Methanamine, compd. with borane (1:1); Methylamine, compd. with BH3 (6CI, 7CI); Methylamine, compd. with borane (1:1) (8CI); Borane-methylamine; Borane-methylamine compound (1:1); Methylamine borane; Monomethylamine-borane	1722-33-4		Not available

Chemical or Trade Name and Synonyms	CAS Registry Number®	Structure	Pharmacological Activities and Additional Comments
Boron, trihydro(2-methyl-2-propanamine)-, (T-4)- 2-Propanamine, 2-methyl-, compd. with borane (1:1); Borane, compd. with 2-methyl-2-propanamine (1:1); Borane, compd. with tert-butylamine (1:1) (8CI); tert-Butylamine, compd. with BH3 (6CI); tert-Butylamine, compd. with BH3 (1:1) (7CI); tert-Butylamine, compd. with borane (1:1) (8CI); (tert-Butylamine)trihydroboron; NSC 114045; tert-Butylamine borane; tert-Butylamine-borane (1:1)	7337-45-3		**oral LD_{50} guinea pig** = 50 mg/kg; additional noted effects: (1) altered sleep time (including change in righting reflex), (2) convulsions or effect on seizure threshold (ChemIDplus, undated-b) **oral LD_{50} mouse** = 25 mg/kg; additional noted effects: muscle weakness (ChemIDplus, undated-b) **oral LD_{50} rat** = 96 mg/kg; additional noted effects: (1) tremors, (2) convulsions or effect on seizure threshold, (3) changes to gastrointestinal tract (ChemIDplus, undated-b) **skin LD_{50} guinea pig** >1000 mg/kg; additional noted effects: (1) dermatitis observed after systemic exposure, (2) effect on animal hair observed (ChemIDplus, undated-b) **skin LD_{50} rabbit** = 820 mg/kg (ChemIDplus, undated-b) **i.p. LD_{50} mouse** = 16 mg/kg (ChemIDplus, undated-b; Hall et al., 1980 [PMID:6251198]) **i.p. LD_{50} rat** = 10 mg/kg; additional noted effects: (1) convulsions or effect on seizure thresholds, (2) ataxia; (3) effect on hair (ChemIDplus, undated-b) Inactive in NCI *In Vivo* Anticancer Drug Screen. Data for tumor model L1210 Leukemia (i.p.) in B6D2F1 (BDF1) mice (PubChem, Undated [CID:24190737]) Inactive in NCI Yeast Anticancer Drug Screen (strains tested: mlh1 rad18, bub3, cln2 rad14, sgs1 mgt1, mec2-1, and rad50 strain) (PubChem, Undated [CID:24190737]) **National Occupational Hazard Survey** Haz. Number Year / Code / Indust. / Facilities / Occup. / Employees 1974 A1308 2 88 2 243 1983 A1308 1 3 1 22

Chemical or Trade Name and Synonyms	CAS Registry Number®	Structure	Pharmacological Activities and Additional Comments
Diborane Boroethane; Boron hydride; Diborane(6); Diboron hexahydride	19287-45-7		**inhalation LC_{50} mouse** = 29 ppm (4 hr); additional noted effects: (1) olfaction, (2) acute pulmonary edema, (3) dyspnea (ChemIDplus, undated-c; HSDB, 2006) **inhalation LC_{50} male mouse** = 31.5 ppm (4 hr) (HSDB, 2006) **inhalation LC_{50} rat** = 40 or 80 ppm (4 hr), depending on age (ChemIDplus, undated-c; HSDB, 2006); 50 ppm (OSHA, undated) Human exposure results in a variety of symptoms, including pulmonary irritation, headaches, dizziness, nausea, coughing, muscle fatigue and weakness, tremors, pulmonary damage/edema, pneumonitis, and potential systemic organ effects on the heart, liver, kidneys, and nervous system. Acute poisoning symptoms are similar to metal fume fever. Diborane is corrosive to the skin, eyes, and respiratory tract. The lethal concentration is 159 ppm (15 min) (HSDB, 2006; OSHA, undated). Acute, short-term, and chronic exposure studies in animals affected mainly the respiratory system. A significant increase in lung weight was observed. Reported observations range from respiratory distress, hypoxia, pulmonary hemorrhage, edema, and death (acute) to pulmonary edema, rhinitis, pneumonia, and structural lung damage (chronic). For mice, an NOEL of 1 ppm for an 8-hr exposure was determined. A reproductive toxicity study in male Wistar rats revealed no effects on the testes (HSDB, 2006). Ames test: negative in *Salmonella typhimurium* strains TA98, TA100, TA1535, and TA1537 ±S9. Gas exposure method: positive in TA98 and TA100 ±S9; negative in TA1535 and TA1537 ±S9; positive in *Escherichia coli* WP2 uvrA +S9 and negative -S9 (CCRIS, 2004)

[1]Morpholine borane (4856-95-5), pyridine borane (110-51-0), and diethylamino-diborane (122703-19-9) were excluded from this evaluation due to the presence of ring moieties which are not present in the parent compound (dimethylamine borane). Cursory search on these chemicals in PubChem and ChemIDplus found toxicological information for morpholine borane and pyridine borane (ChemIDplus, undated-d; ChemIDplus, undated-e).

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CCRIS (Chemical Carcinogenesis Research Information System). 2004. Diborane. CCRIS Record No. 4780. Internet address: http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+ccris:@term+@rn+19287-45-7. Profile last updated on October 12, 2004. Last accessed on July 16, 2008.

ChemIDplus. Undated-a. Boron, (N,N-dimethylmethanamine)trihydro-, (T-4)-; RN: 75-22-9. Internet address: http://chem.sis.nlm.nih.gov/chemidplus/ [searched by Registry Number]. Last accessed on July 16, 2008.

ChemIDplus. Undated-b. Boron, trihydro(2-methyl-2-propanamine)-, (T-4)-; RN: 7337-45-3. Internet address: http://chem.sis.nlm.nih.gov/chemidplus/ [searched by Registry Number]. Last accessed on July 16, 2007.

ChemIDplus. Undated-c. Diborane; RN: 19287-45-7. Internet address: http://chem.sis.nlm.nih.gov/chemidplus/ [searched by Registry Number]. Last accessed on July 16, 2008.

ChemIDplus. Undated-d. Boron, trihydro(morpholine-kappaN4)-, (T-4)-RN: 4856-95-5. Internet address: http://chem.sis.nlm.nih.gov/chemidplus/ [searched by Registry Number]. Last accessed on September 20, 2007.

ChemIDplus. Undated-e. Pyridine borane; RN: 110-51-0. Internet address: http://chem.sis.nlm.nih.gov/chemidplus/ [searched by Registry Number]. Last accessed on September 20, 2007.

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OSHA (Occupational Safety and Health Administration). Undated. Occupational Safety and Health Guideline for Diborane. U.S. Department of Labor, OSHA, Washington, DC. Internet address: http://www.osha.gov/SLTC/healthguidelines/diborane/recognition.html/. Last accessed on July 16, 2008.

PubChem. Undated. Compound Summary for the following compounds (see BioActivity Summary):

- Trimethylamine borane. Internet address: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=6327651&loc=ec_rcs. Last accessed on July 16, 2008.
- tert-Butylamine borane. Internet address: http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=24190737&loc=ec_rcs. Last accessed on June 27, 2008.