



DBDCB

DATE: 08/18/20069

CAS NO: 3591-65-7

SUPERSEDES: 01/01/2003

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME: DBDCB
SYNONYMS: 1,2-Dibromo-2,4-Dicyanobutane
CHEMICAL FAMILY: Brominated Organic
MOLECULAR FORMULA: C₆H₆N₂Br₂
MOLECULAR WEIGHT: 266

VERICHEM, 3499 Grand Avenue, Pittsburgh, PA, USA, 15225 (412-331-7299, 8:30 am to 5:00 pm)
EMERGENCY PHONE: For any emergency involving spill, leak, fire, exposure, or accident call
CHEMTREC: 1-800-424-9300. Outside the USA and Canada call: 703-527-3887

2. COMPOSITION/INFORMATION ON INGREDIENTS

REGULATED COMPONENTS

COMPONENT	CAS NUMBER	PERCENT	WORKER EXPOSURE	REFERENCE
1,2,-Dibromo-2,4-dicyanobutane	35691-65-7	98		

3. HAZARDS IDENTIFICATION

EMERGENCY OVERVIEW

APPEARANCE AND ODOR: White crystalline powder.

EFFECTS OF OVEREXPOSURE **DANGER. CORROSIVE** Causes irreversible eye damage. May be fatal if inhaled. Harmful if swallowed or absorbed through skin. Do not get in eyes, on skin or on clothing. Wear goggles, safety glasses or face shield when handling. Avoid contact with skin. Do not breathe vapor or spray mist dust. Prolonged or frequently repeated skin contact may cause allergic reaction in some individuals. Remove contaminated clothing and wash clothing before reuse.

HUMAN: Irritating to skin and eyes

ENVIRONMENTAL: Toxic to fish

4. FIRST AID MEASURES (IN CASE OF CONTACT):

IF IN EYES: Hold eyes open and rinse slowly and gently with water for 15-20 minutes. Get medical attention. Remove contact lenses, if present, after the first 5 minute, then continue rinsing eye. Call a poison control center or doctor for treatment advice.

IF ON SKIN: Take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 minutes. Call a poison control center or doctor for treatment advice.

IF SWALLOWED: Call a poison control center or doctor immediately for treatment advice. Have a person sip a glass of water if able to swallow. Do not induce vomiting unless told to do so by a poison control center or doctor. Do not give anything by mouth to an unconscious person.

IF INHALED: Move person to fresh air. If not breathing, call 911 or an ambulance, then give artificial respiration, preferably mouth-to-mouth. Call a poison control center or doctor for treatment advice.

Have the product container or label with you when calling a poison control center or doctor, or going for treatment.

NOTE TO PHYSICIAN: Probable mucosal damage may contraindicate the use of gastric lavage.

5. **FIRE FIGHTING MEASURES**

FLAMMABLE PROPERTIES

This product is not by definition a “flammable liquid” or a “combustible liquid”.

FLASH POINT:

Not Flammable

FLAMMABLE LIMITS (% BY VOLUME):

Not Applicable

AUTOIGNITION TEMPERATURE:

Not Applicable

DECOMPOSITION TEMPERATURE:

>50° C

EXTINGUISHING MEDIA AND FIRE FIGHTING INSTRUCTION

FIRE HAZARDS

Product is not flammable. If product is involved with other substances, use water, dry chemical or CO₂. Exercise caution when fighting fires involving chemical substances. Respiratory protection is required. As in any fire, prevent human exposure to fire, smoke, fumes, or products of combustion. Evacuate nonessential personnel from the fire area. Fire fighters should wear full face, self -contained breathing apparatus and impervious protective clothing. Use standard fire-fighting techniques to extinguish fires involving this material. Use water spray, Dry chemicals, foam or carbon dioxide. If drums are NOT leaking, keep fire-exposed containers cool with a water spray to prevent rupture due to excessive heat. High-pressure water hoses may spread product from broken containers, increasing contamination or fire hazards. Contaminated buildings, areas and equipment must not be used until they are properly decontaminated. If fire cannot be controlled and containers are heated, **EVACUATE THE AREA!**

6. **ACCIDENTAL RELEASE MEASURES**

STEPS TO BE TAKEN IN CASE MATERIAL IS RELEASED OR SPILLED

Immediately dyke material to keep away from water sources. Scoop up material. Residual amounts left on surfaces may be cleaned with soap and water. Rinse residuals to municipal treatment plant.

7. **HANDLING AND STORAGE**

Handling: Keep container closed when not in use. Store out of heat. Material melts at temperature >50° C.

8. **PERSONAL PROTECTION**

EYE PROTECTION REQUIREMENTS: Protective eye wear. **SKIN PROTECTION REQUIREMENTS:**

Coveralls worn over long-sleeved shirt and long pants, socks, chemical-resistant footwear and gloves.

VENTILATION REQUIREMENTS: Use local exhaust ventilation where dust or vapor may be generated.

RESPIRATOR REQUIREMENTS: Respiratory protection device.

9. **PHYSICAL AND CHEMICAL PROPERTIES**

APPEARANCE AND ODOR: White crystalline Powder

BOILING POINT: Not Applicable

MELTING POINT: 51° C - 53° C

VAPOR PRESSURE: Negligible

SPECIFIC GRAVITY: 2.02

VAPOR DENSITY: Not Applicable

PERCENT VOLATILE (BY WEIGHT): 0

pH: Not Applicable

SATURATION IN AIR (PERCENT BY VOLUME): Not Applicable

EVAPORATION RATE: Not Applicable

SOLUBILITY IN WATER: 2300 ppm at 25° C

10. **STABILITY AND REACTIVITY**

STABILITY: Stable

POLYMERIZATION : will not occur

INCOMPATIBLE MATERIALS: Strong Oxidizers, Bases

HAZARDOUS DECOMPOSITION PRODUCTS: Bromine, 1,2-Dicyano-1-Butene HBr

CONDITIONS TO AVOID: Excessive heat; Store less than 45°C

11. **TOXICOLOGICAL INFORMATION**

ACUTE EFFECTS:

LD₅₀ (oral rat) 705 mg/kg
LD₅₀ (oral mouse) 530 mg/kg
LD₅₀ dermal rabbit >5.0 g/kg
LC₅₀ (inhalation –1hr –rat)>200 mg/l

EYE: Primary Eye Irritation: Testing done on rabbits indicates that DBDCB (as is) is a severe eye irritant. For the unwashed and washed eyes, corneal, iridal, and conjunctival effects were noted. A wash after 4 seconds did not ameliorate the gross effects. Testing done on a 0.2% solution (2000 ppm) on rabbits that the material produced no corneal opacity or iritis, but moderate conjunctival irritation was present in 3 out of 6 eyes which improved by day 3. Testing conducted on a 0.1% solution (1000 ppm) on rabbits showed the material produced no corneal, iridal, or conjunctival effects on any of the animals.

SKIN CONTACT: Primary Skin Irritation Index: The product (as is) was found to produce moderate irritation to rabbit skin. Further testing conducted on rabbits at a concentration of 0.3% (3000 ppm) resulted in minimal skin irritation. Primary irritation index was 0.5/8.

D.O.T. Corrosivity Testing: Six rabbits dosed with 0.5 g of the material. The product was applied to intact skin and kept in contact for 4 hours. Scores were made at 4 and 48 hours after application. The material was not found to be corrosive.

SENSITIZATION: Animal Testing: DBDCB was tested on guinea pigs by both a modified Ritz/Buehler method as well as modified Magnusson-Kligman maximization method. In neither test did the product produce any irritation or sensitization reactions.

Repeated Human Insult Patch Test. Product has been tested at 3000 ppm using a modified Shelanski technique on 106 participants. None of the participants tested were sensitized to the test material. An additional test, again using the Shelanski technique, used 52 panelists applying material at 3000 ppm in corn oil. Again, the material was not a sensitizing agent. DBDCB, using a modified Draize technique, was tested in both petrolatum and ethanol at 5000 ppm concentration. At the 5000 ppm concentration the material appeared to produce some cumulative irritation. The ethanol patch sites were more reactive than the petrolatum patch sites. In one study only the petrolatum vehicle containing the DBDCB was employed as the challenge. In the other studies a nonionic cream was used as the challenge. During both studies the material appeared to produce some sensitizing.

SUBCHRONIC EFFECTS

13 Week Dietary Study (rats)

The effect of DBDCB when administered in the diet of rats for a 13 week period was evaluated in this study. The chemical was added to the rats' diet at levels of 83.5, 500 and 3000 ppm. No dose related effects for clinical laboratory data and gross pathology were noted at 83.5 and 500 ppm levels. A reduction of body weight gain was noted at the 3000 ppm level together with slight changes in the spleen (extramedullary hematopoiesis in females). No other dose-related effects were noted at the highest level tested.

13-Week Dietary Study (dogs)

In order to assess the long-range effects of dietary intake of small amounts of DBDCB through indirect food additive applications, a 13-week subchronic dietary study was completed using Beagle dogs. The chemical was added to the dogs' diet at levels of 167, 1000 and 4000 ppm. The no-effect level was found to be >1000 ppm. In the highest level tested, 4000 ppm, reduction in the food consumption and body weight gain was noted as well as changes in the thyroid gland (increase follicular cell height or hyperplasia). No other dose-related effects were noted in this study.

13-Week Thyroid Function Study in Dogs

The material was administered to dogs at a dose level of 167 ppm over a 13 week period. Basal and thyroid stimulated hormone levels of triiodothyronine and thyroxine were determined for all dogs prior to the study and/or during the treatment. No compound-related differences were noted between control and treated dogs (167 ppm) in clinical observation: body weights; food consumption; basal, stimulated, or fold increases of T3 and T4; histopathological alterations. Increased thyroid and thyroid to body weight ratio were noted in the treated females when compared to the control, but not in treated males.

Pharmacokinetic Study in Rats

The excretion of ¹⁴C DBDCB following a single oral administration in male rats was investigated with respect to three excretory pathways, namely: urinary, fecal and respiratory. Respired ¹⁴CO₂ comprised about 0.5% of the total administered dose in both rats during the 32 hour period following compound administration.

Oral dosing of rats with ¹⁴C DBDCB showed that 6-10% of the total administered dose was excreted in the feces during a 168-hour collection period. The greatest amount (60-80%) of the total fecal excretion occurred in the final 48 hours of sample collection.

Urinary excretion was the major route of elimination in the rat. Between 84 and 91% of the total administered dose was excreted in the urine, mostly in the first 24 hours of sample collection.

An analysis of organs for radiotracer content showed that, by 168 hours after administration, very little was found. 0.3% of the administered radioactivity remained in the liver while <0.1% of the total dose was detected in all other organs surveyed (kidneys, adrenals, thymus, spleen, heart, lungs, testes, brain, mesenteric fat and muscle).

The maximum blood concentration (~7/ug/ml) of ¹⁴C DBDCB and/or its metabolites in whole blood was attained at about 5 hours post administration.

¹⁴C DBDCB concentration in plasma following oral administration is roughly equivalent to concentrations in the whole blood - up to 24 hours postadministration. The concentrations of compound in plasma at a later time (≥24 hours) are less than in the whole blood. Total concentration in the blood was low at all times.

GENOTOXIC EFFECTS

Ames Test

DBDCB was evaluated as a potential mutagen using any Ames-type procedure with various histidindependent strains of the bacteria Salmonella typhimurium. Specific strains tested were TA1537, TA1535, TA98, and TA100. Product was found to be non-mutagenic.

In Vitro Cytogenicity Using Chinese Hamster Ovary Cells

The product was tested at 9 doses with metabolic activation and 8 dose levels without activation. The chromosome aberrations were scored and evaluated at 3 doses.

The results of the assay indicate that under conditions of the test, the test material causes a significant increase in the frequency of chromosome aberration in Chinese Hamster Ovary cells, with and without S-9 activation. A difference in the test article between the activated and non-activated systems was observed. It appears the differential toxicity may be due to the

detoxification of the test material by the S-9 mix. Additional studies were conducted using the In Vivo method to further clarify the results.

In Vivo Cytogenicity Using Sprague-Dawley Rats

Male Sprague-Dawley rats were exposed by gavage to 3 dose levels (50 mg/kg, 17 mg/kg 5 mg/kg) of product for 5 consecutive days. Bone marrow cells arrested in metaphase and collected approximately 24 hours after the last dose administration were examined microscopically for chromosome aberrations, both numerical and structural. The results of the assay indicate that under conditions described in the report, the test material did not induce a significant increase in chromosome aberrations in male rats.

Modified Dominant Lethal Evaluation Using Mice

This study was carried out in male mice at levels up to and including 3000 ppm of DBDCB in the diet. These mice were then mated with female mice who were not exposed to the chemical and the number and condition of each fetus examined for signs of genetic damage. This test also indicates any sterilizing properties of the chemical to the male mice. Under these conditions, no sterility or dominant lethal mutations were noted at any of the levels of DBDCB used.

Unscheduled DNA Synthesis in Human IMR-90 Fibroblasts

DBDCB did not induce UDS in human cells at any dose level. DBDCB produced a significant reduction in tritiated thymidine incorporated at all dose levels with S-9 activation at 10 ug/ml and 0.1 ug/ml without activation.

Teratology

Female rats were mated and administered DBDCB to assess the teratogenic potential. The test article was administered orally by gavage from days 6 through 15 of gestation at dose levels of (control), 25, 100, or 175 mg/kg.

No pharmacological signs of maternal toxicity were observed. The findings of this study indicate that DBDCB was not embryotoxic or teratogenic at dose levels up to 175 mg/kg (highest level treated).

12. ECOLOGICAL INFORMATION**ENVIRONMENTAL FATE:****ACTIVATED SLUDGE**

A study was run to determine the effects of DBDCB on nine waste treatment process. The microorganisms were exposed to increasing concentrations of DBDCB over ten days. DBDCB did not have a significant effect on the microbial population. Bacterial and fungal populations remain viable during the test period DBDCB concentrations from 0.1 to 99 ppm. At the treatment levels tested, the DBDCB was completely metabolized with one day. At lower concentrations DBDCB was metabolized to radio labeled CO₂. At higher concentrations (>5 ppm) the C¹⁴, was found primarily in the liquid phase and was determined to be Methylene glutaronitrile.

ENVIRONMENTAL CHEMISTRY:**WILDLIFE****Eight-day Feeding Study-Mallard Duck**

The acute LC₅₀ of Tektamer 38 was found to be >10,000 ppm.

Eight-day Feeding Study-Bobwhite Quail

The LC₅₀ was found to be 4042 ppm.

Acute Oral LD₅₀ -Mallard Duck

The LD₅₀ was found to be 1064 mg/kg.

FISH/INVERTEBRATES

LC₅₀-Bluegill Sunfish (96 hrs.)-4.09 mg/l.

LC₅₀-Rainbow Trout (96 hrs.)-1.75 mg/l.

LC₅₀-Sheepshead Minnows (96 hrs.)-17 mg/l.

LC₅₀-Daphnia magna (48 hrs.)-2.2 mg/l.

LC₅₀-Grass Shrimp (48 hrs.)-45 mg/l.

LC₅₀-Blue Crabs (96 hrs.)->1000 mg/l.

13. DISPOSAL CONSIDERATION

PROHIBITIONS: Do not contaminate water, food or feed by storage or disposal.

PESTICIDE DISPOSAL: Pesticide wastes are acutely hazardous. Improper disposal of excess pesticide or rinsate is a violation of Federal Law. If waste cannot be disposed of by use according to label instructions, contact your State Pesticide or Environmental Control Agency or the Hazardous Waste representative at the nearest EPA Regional Office for guidance. **CONTAINER DISPOSAL:** Do not reuse empty container. Triple rinse (or equivalent). Then offer for recycling or reconditioning, or puncture and dispose of in a sanitary landfill, or by other procedures approved by the state and local authorities.

14. TRANSPORT INFORMATION

This section provides basic shipping classification information. Refer to appropriate transportation regulations for specific requirements.

	DOT Shipping Information	IMO Shipping Information	ICAO/IATA	TRANSPORT CANADA
Shipping Name	DBDCB	DBDCB	DBDCB	DBDCB
Hazard Class	Not Restricted	Not Restricted	Not Restricted	Not Restricted
Packing Group	N/A	N/A	N/A	N/A
Subsidiary Class		N/A	N/A	N/A
UN/ID Number	N/A	N/A	N/A	N/A
Transport Label Required	N/A	N/A	N/A	N/A
Packing Instructions Passenger Cargo	N/A	N/A	N/A	N/A
Max. Net Quantity Passenger Cargo	N/A	N/A	N/A	N/A
D.O.T. Hazardous Substances	N/A	N/A	N/A	N/A
IMDG Page	N/A	N/A	N/A	N/A

15. REGULATORY INFORMATION

INVENTORY INFORMATION

US TSCA: Yes

CANADA DSL: Yes

EEC EINECS: Yes

COMPONENT:

CAS. NUMBER: 35691-65-7

PERCENT: 98%

16. OTHER INFORMATION

NFPA HAZARD RATING (NATIONAL FIRE PROTECTION ASSOCIATION)

FIRE: 0

HEALTH: 2

REACTIVITY: 1

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