3.0 PHYSICAL AND CHEMICAL PROPERTIES AND ANALYTICAL METHODS

PRINCIPAL FINDINGS

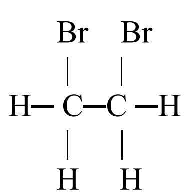
- Both EDB and EDC:
    - are more soluble in water than BTEX, but less soluble than MTBE.
    - are less volatile than BTEX or MTBE.
- EDB
    - can be detected at or below its maximum contaminant level (MCL) of 0.05 μg/L using EPA Methods 8011 or 504.1.
- EDC:
    - can be detected at or below its MCL of 5 μg/L using EPA Methods 8260B, 502.2, 504.1, or 524.2.

3.1 PHYSICAL AND CHEMICAL PROPERTIES

This section provides information about select physical and chemical properties of EDB and EDC in comparison to each other and to other common components of gasoline such as benzene, toluene, ethylbenzene, and xylene (BTEX) and methyl tert-butyl ether (MTBE). Table 3-1 identifies commonly used synonyms and trade names for EDB and EDC. Some of the important physical and chemical properties of EDB, EDC, BTEX, and MTBE are listed in Table 3-2.

The molecular structures of EDB and EDC are depicted below.

EDB ($C_2H_4Br_2$)



EDC ($C_2H_4Cl_2$)

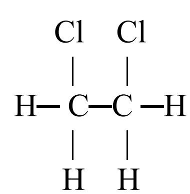


Table 3-1: Synonyms and Trade Names for EDB and EDC

Chemical	Synonyms	Trade Names
EDB	Ethylene dibromide; 1,2-dibromoethane; dibromoethane; ethylene bromide; ethane,1,2-dibromo; α-, β-dibromoethane; sym-dibromoethane; glycol bromide; glycol dibromide	Bromofume; Dowfume W85; Dowfume EDB; Dowfume 40, W-10, W-40; Dowfume MC-2; Iscobrome D; ENT 15; 349; Netis; Pestmaster EDB-85; Santryum; unifume; EDB-85; Fumogas; Icopfume soilbrom-85; soilfume
EDC	Ethylene dichloride; 1,2-dichloroethane; dibromoethane; ethane,1,2-dichloro; α-, β-dichloroethane; sym-dichloroethane	Freon 150; Borer sol; Brocide; Destruxol borer-sol; Dichlor-mulsion; Dutch liquid; Dutch oil; ENT 1656, Gaze Olefiant; Granosan

Source: Refs. 3-1, 3-2, 3-3, 3-15, and 3-16

The following relative physical properties of EDB, EDC, BTEX, and MTBE are depicted in Figures 3-1 through 3-6:

- Specific gravity
- Water solubility
- Log K_{ow} (octanol-water partition coefficient)
- Vapor pressure
- Log K_{oc} (soil organic carbon/water partition coefficient)
- Henry's law constant

Key findings about the physical properties of EDB and EDC include the following:

- The specific gravities of EDB and EDC are higher than those of BTEX and MTBE.
- EDB and EDC are more soluble in water than BTEX and less soluble than MTBE. The solubilities of EDB and EDC are 4,200 and 8,310 milligrams per liter (mg/L), respectively.
- EDB and EDC are more soluble in water and less soluble in oil than BTEX.
- EDB and EDC are less soluble in water and more soluble in oil than MTBE.
- EDB and EDC vaporize more slowly than benzene, toluene, and MTBE.
- EDB and EDC bind less easily to soil than BTEX.
- EDB and EDC bind more easily to soil than MTBE.

Table 3-2: Physical and Chemical Properties of Selected Gasoline Components-Lead Scavengers (EDB and EDC), BTEX, and MTBE

Chemical	Physical Description [1]	Molecular Structure	Molecular Weight (g/mol)	Specific Gravity	Boiling Point (°C)	Water Solubility (mg/L)	Log K_{ow}	Vapor Pressure at 25 °C (mm Hg)	Log K_{oc}	Henry's Law Constant (dimensionless)
EDB	Colorless liquid with a mild, sweet odor	CH_2Br-CH_2Br	187.88	2.17 [1]	131.3 [1]	4,200 [4]	1.74 [4]	11 [1]	1.45 [4]	0.0133 [4]
EDC	Colorless, oily, organic liquid with a sweet, chloroform-like odor	CH_2Cl-CH_2Cl	98.97	1.24 [1]	83.5 [1]	8,310 [4]	1.47 [4]	12 [1]	1.58 [4]	0.0401 [4]
Benzene	Colorless to light-yellow liquid with an aromatic odor	C_6H_6	78.11[3]	0.88 [3]	80.1[3]	1,780 [3]	2.13 [3]	76 [3] 95.2 [3]	1.8-1.99 [3] 1.5 - 2.16 [3]	0.2219 [3]
Toluene	Colorless liquid with a sweet, pungent, benzene-like odor	$C_6H_5CH_3$	92.13 [3]	0.87 [3]	110.6 [3]	534.8 [3]	2.73 [3]	28.4 [3]	1.56-2.25 [3]	0.2428 [3]
Ethylbenzene	Colorless liquid with an aromatic odor	$CH_3CH_2C_6H_5$	106.16[3]	0.87 [3]	136.25 [3]	161 [3]	3.15 [3]	9.53 [3]	2.94 [3] 1.98-3.04 [3]	0.345 [3]
Xylene m-Xylene o-Xylene p-Xylene	Colorless liquid with an aromatic odor	$C_6H_4(CH_3)_2$	106.16 [3] 106.16 [3] 106.17 [3]	0.8842 [3] 0.8802 [3] 0.8611[3]	139.03 [3] 144.4 [3] 137-138[3]	146 [3] 175 [3] 156 [3]	3.20 [3] 3.12 [3] 3.15 [3]	8.3 [3] 6.6 [3] 8.7 [3]	2.04-3.15 [3] 1.68-1.83 [3] 2.05-3.08 [3]	0.3139 [3] 0.0208 [3] 0.3139 [3]
MTBE	Clear liquid with a turpene-like odor	CH_3-O-$C(CH_3)_3$	88.15 [2]	0.74 [2]	55.2 [2]	43,000 - 54,300 [2]	1.06 [2]	245-256 [2]	1.0-1.1 [2]	0.024-0.12 [2]

Notes:
(1) Data from Ref. 3-3
(2) Data from Ref. 3-5
(3) Data from Ref. 3-17
(4) Data from Ref. 3-4

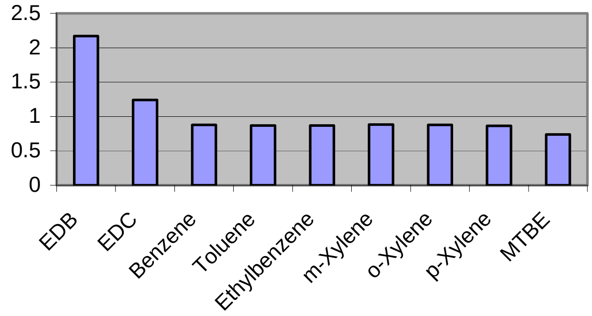


Figure 3-1. Relative Specific Gravities of EDB, EDC, BTEX, and MTBE

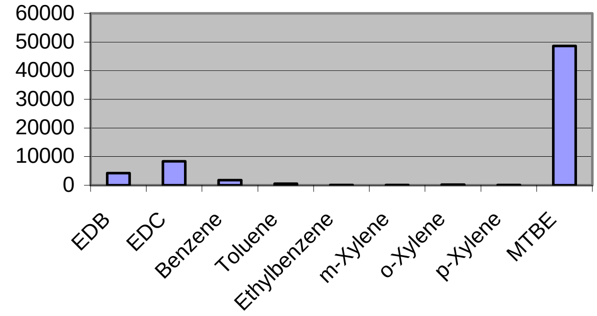


Figure 3-2. Relative Water Solubility (mg/L) of EDB, EDC, BTEX, and MTBE

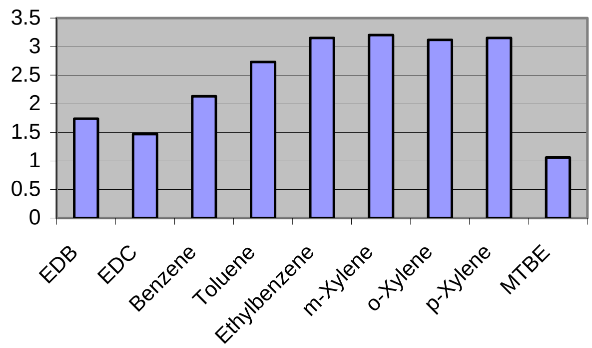


Figure 3-3. Relative Log $K_{ow\,*}$ of EDB, EDC, BTEX, and MTBE

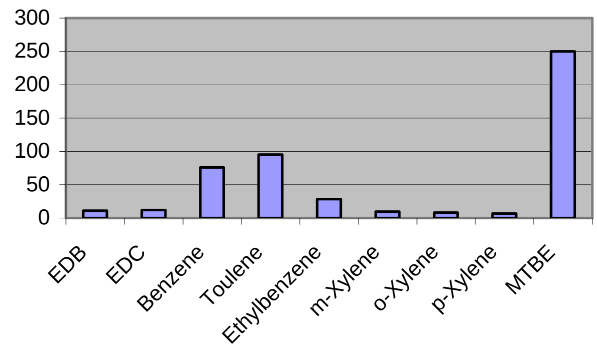


Figure 3-4. Relative Vapor Pressure (mm Hg) of EDB, EDC, BTEX, and MTBE

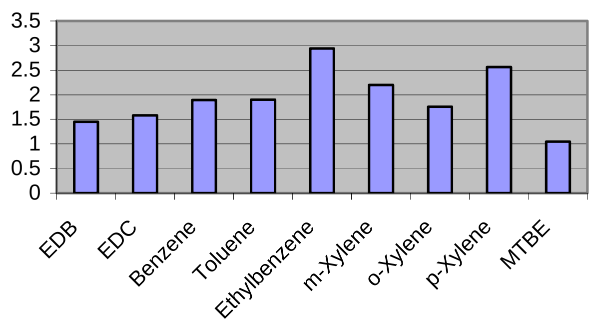


Figure 3-5. Relative Log $K_{oc\,+}$ of EDB, EDC, BTEX, and MTBE

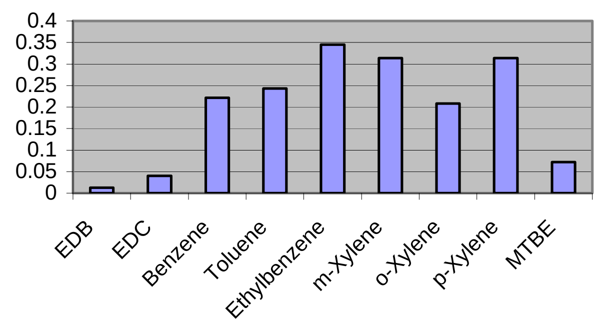


Figure 3-6. Relative Henry's Law Constants of EDB, EDC, BTEX, and MTBE

Notes
* **Octanol-water partition coefficient**
\+ **Soil organic carbon/water partition coefficient**

Source: Refer to Table 3-2.

3.2 ANALYTICAL METHODS FOR EDB AND EDC

This section summarizes the analytical methods for EDB and EDC in soil, hazardous waste, and groundwater as well as in drinking water. Groundwater used as a drinking water source must be analyzed using EPA-specified methods for drinking water.

3.2.1 Soil, Hazardous Waste, and Groundwater

EDB and EDC are listed constituents of many hazardous wastes.

- In 40 CFR 261.24, EDC is a toxicity characteristic waste with EPA Hazardous Waste (HW) No. D028. Also, 40 CFR 261.31, "Hazardous Wastes from Non-specific Sources," includes EDC under HW Nos. F024 and F025.
- In 40 CFR 261.32, "Hazardous Wastes from Specific Sources," EDC is included under HW Nos. K018, K019, K020, K029, K030, and K096, and EDB is included under HW Nos. K117, K118, and K136.
- In 40 CFR 261.33, "Discarded Commercial Products, Off-specification Species, Container Residues, and Spill Residue Thereof," EDC is included as HW No. U077, and EDB is included as HW No. U067.
- EDB and EDC are listed in Appendix VIII, "Hazardous Constituents," to 40 CFR 261. Also, both EDB and EDC are included on the "Skinner List" of hazardous constituents associated with petroleum facilities.

SW-846, "Test Methods for Evaluating Solid Waste, Physical/Chemical Methods," is EPA's official compendium of analytical and test methods that have been evaluated and found to be acceptable under Subtitle C of the Resource Conservation and Recovery Act (RCRA), as amended. SW-846 describes a wide range of methodologies and can be accessed online at *http://www.epa.gov/SW-846/sw846.htm* (Ref. 3-14). Table 3-3 identifies SW-846 methods that can be used for EDB and EDC analyses.

Methods 8011 and 8021B are used for EDB analysis of wastes, soils, and similar media. Method 8260B is used for EDC analysis of wastes, soils, and similar media. Alternative methods for EDC analysis include those used for EDB and Method 8261, which uses a preliminary vacuum distillation step.

Table 3-3: Summary of EPA Analytical Methods for EDB and EDC in Soil, Hazardous Waste, and Groundwater

Chemical	EPA Method Number	Determinative Method Name	Method Detection Limit (µg/L)	Preparation Method Name	
				SW-846 Method Number	SW-846 Method Name
EDB	8011	Microextraction and Gas Chromatography with Electron Capture (Ref. 3-6)	0.01	8011	Direct Injection
	8021B	Gas Chromatography Using Photoionization and/or Electrolytic Conductivity Detectors (Ref. 3-7)	0.8	5030B	Purge-and-Trap
				5021	Head Space
	8260B	Volatile Organic Compounds Gas Chromatography/Mass Spectrometry (Ref. 3-6)	0.06	5030B/ 5035	Purge-and-trap
				5021	Head Space
EDC	8260B	Volatile Organic Compounds Gas Chromatography with Halogen-Specific Detectors (Ref. 3-8)	0.02	5030B/ 5035	Purge-and-Trap
				5032	Vacuum Distillation
				5021	Head Space
	8261	Vacuum Distillation in Combination with Gas Chromatography/Mass Spectrometry (Ref. 3-9)	0.1	8261	Distillation and Trap

Source*:* Ref. 3-14

3.2.2 Drinking Water

Periodic sampling and analysis of community water supplies for EDB and EDC (and other specified organic compounds) must be performed using the methods specified in 40 CFR 141.24 or other methods that have been demonstrated to be equivalent.

For EDC, the specified drinking water analytical methods are EPA Methods 502.2 and 524.2, both of which are general methods for many volatile organic compounds (VOC). Both methods use purge-and-trap introduction to a capillary column gas chromatography system. Method 502.2 uses photoionization and electrolytic conduction detectors in series, and Method 524.2

uses a mass spectrometry detector. Method 502.2 provides better sensitivity (a lower detection limit), whereas Method 524.2 provides independent confirmation of an analyte's identity. EDC can also be analyzed by using method 504.1.

Due to the low maximum contaminant level (MCL) of EDB (0.05 µg/L) two additional, specialized EPA methods for EDB analysis have been developed. Method 504.1 is similar to Method 502.2 but includes a preliminary extraction and concentration step to provide lower sample detection limits. Method 551.1 is similar to Method 504.1 but uses a different preliminary extraction technique that has been adapted to cover a wider variety of halogenated organic compounds. Table 3-4 summarizes the EPA analytical methods for EDB and EDC in drinking water.

Table 3-4: Summary of EPA Analytical Methods for EDB and EDC in Drinking Water

Chemical	EPA Method Number	Method Name	Method Detection Limit (µg/L)	MCL (µg/L)
EDB	504.1	Microextraction and Gas Chromatography (Ref. 3-11)	0.01	0.05
	551.1	Liquid-Liquid Extraction and Gas Chromatography with Electron Capture (Ref. 3-13)	0.032	
EDC	502.2	Purge-and-Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series (Ref. 3-10)	0.03	5
	504.1	Microextraction and Gas Chromatography with Electron Capture (Ref. 3-11)	0.01	
	524.2	Purge-and-Trap Gas Chromatography/Mass Spectrometry (Ref. 3-12)	0.06	

Source: Ref. 3-14

3.2.3 Method Adequacy

Selection of the appropriate analytical method for EDB or EDC is primarily based on the method detection limit and the intended use of the analytical data.

Analysis of some samples with high concentrations of total VOCs (such as samples containing significant quantities of gasoline) may require dilutions so that the sample detection limits are above the MCLs or risk-based limits[1] used as cleanup goals. This consideration is more relevant

[1] Various EPA regions define risk-based limits using different terminology. For example, EPA Region 3's risk-based limits are called risk-based concentrations and can be obtained from http://www.epa.gov/reg3hwmd/risk/rbc0403.pdf. EPA Region 9's risk-based limits are called preliminary remediation goals and can be obtained from

to EDB because of its lower MCL and risk-based limits. It is usually possible to work around the detection limit concerns by choosing the proper analytical method. In particular, electrolytic conductivity detectors such as those used in Methods 502.2, 504.1, 8011, and 8021B provide strong responses to halogen-containing compounds but little or no response to hydrocarbons.

Another potential problem arises when a sample has a relatively high concentration of a compound that produces a large chromatographic peak near the peak produced by EDB or EDC. In this case, the tail of the large peak may mask the EDB or EDC peak. This problem can often be overcome by adjusting the chromatographic conditions to separate the peaks.

3.3 REFERENCES

3-1 Agency for Toxic Substances and Disease Registry (ATSDR). 1992. Toxicological Profile for 1,2-Dibromoethane. U.S. Department of Health and Human Services, Public Health Service.

3-2 ATSDR. 2001. Toxicological Profile for 1,2-Dichloroethane. U.S. Department of Health and Human Services, Public Health Service.

3-3 National Institute for Occupational Safety and Health (NIOSH). 1997. "Pocket Guide to Chemical Hazards." U.S. Department of Health and Human Services, Public Health Service, Centers for Disease Control and Prevention. Cincinnati, Ohio.

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3-5 EPA. 2004. "Technologies for Treating MTBE and Other Fuel Oxygenates." May.

3-6 EPA. 1992. Test Method 8011 for 1,2-Dibromoethane and 1,2-Dibromo-3-Chloropropane by Microextraction and Gas Chromatography. July.

3-7 EPA. 1996. Test Method 8021B for Aromatic and Halogenated Volatiles by Gas Chromatography Using Photoionization and/or Electrolytic Conductivity Detectors. December.

3-8 EPA. 1996. Test Method 8260B for Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry. December.

3-9 EPA. 2000. Test Method 8261 for Volatile Organic Compounds by Vacuum Distillation in Combination with Gas Chromatography/Mass Spectrometry. November.

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3-10 EPA. 1995. Test Method 502.2 for Volatile Organic Compounds in Water by Purge-and-Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series.

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3-12 EPA. 1995. Test Method 524.2 for Measurement of Purgeable Organic Compounds in Water by Capillary Column Gas Chromatography/Mass Spectrometry.

3-13 EPA.1995. Test Method 551.1 for Determination of Chlorination Disinfection By-products, Chlorinated Solvents, and Halogenated Pesticide/Herbicide in Drinking Water by Liquid-Liquid Extraction and Gas Chromatography with Electron Capture Detection.

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3-15 EPA. 2004. Technical Fact Sheet on Ethylene Dibromide. Website Accessed on September 17, 2004. Online Address: http://www.epa.gov/safewater/dwh/t-soc/edb.html

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