

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of bromoform and dibromochloromethane is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of bromoform and dibromochloromethane is located in Table 4-2.

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Table 4-1. Chemical Identity of Bromoform and Dibromochloromethane

Characteristic	Bromoform	Dibromochloromethane	Reference
Synonyms	Tribromomethane; methenyltribromide; methane, tribromo-	Chlorodibromomethane dibromochloromethane; methane, dibromochloro-; methane, chlorodibromo-	HSDB 2004a, 2004b
Registered trade name(s)	No data	No data	
Chemical formula	CHBr ₃	CHBr ₂ Cl	O'Neil et al. 2001
Chemical structure	$\begin{array}{c} \text{Br} \\ \\ \text{Br}-\text{C}-\text{Br} \\ \\ \text{H} \end{array}$	$\begin{array}{c} \text{Br} \\ \\ \text{Cl}-\text{C}-\text{Br} \\ \\ \text{H} \end{array}$	
Identification numbers:			
CAS registry	75-25-2	124-48-1	O'Neil et al. 2001
NIOSH RTECS	PB5600000	PA6360000	RTECS 2003
EPA hazardous waste	U225	No data	RTECS 2003
OHM/TADS	No data	No data	HSDB 2004a, 2004b
DOT/UN/NA/IMCO shipping	UN2515; IMCO 6.1	No data	HSDB 2004a, 2004b
HSDB	2517	2763	HSDB 2004a, 2004b
NCI	C55130	C55254	RTECS 2003
Beilstein reference number	1731048	1731046	RTECS 2003
Beilstein handbook reference	4-01-00-00082	4-01-00-0081	RTECS 2003
Wisesser line notation	EYEE	GYEE	RTECS 2003

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Bromoform and Dibromochloromethane

Property	Bromoform	Dibromochloromethane	Reference
Molecular weight	252.73	208.28	O'Neil et al. 2001
Color	Colorless	Colorless to pale yellow	Verschueren 2001
Physical state	Liquid	Liquid	Verschueren 2001
Melting point	8.0 °C	-20 °C	Lide 2000
Boiling point	149.1 °C	120 °C	Lide 2000
Density at 20 °C	2.899	2.451	Lide 2000
Odor	Sweet, similar to chloroform	No data	Verschueren 2001
Taste	Similar to chloroform	No data	Lewis 1997
Odor threshold:			
Water	0.51 mg/L	No data	Amoore and Hautala 1983
Air	13.45 mg/m ³	No data	Amoore and Hautala 1983
Solubility:			
Water	3.10x10 ³ mg/L (25 °C)	2.7x10 ³ mg/L (20 °C)	Horvath 1982; Heikes 1987
Organic solvents	Miscible in ethanol, benzene, petroleum ether, acetone, oils	Soluble in ethanol, ether, acetone	Lide 2000
Corrosivity	Will attack some forms of plastics, rubber, and coatings.	No data	HSDB 2004a
Partition coefficients:			
Log octanol/water	2.4	2.16	CITI 1992; Sangster 1994
Log K _{oc}	2.06	1.92	Mabey et al. 1982
Vapor pressure at 20 °C	5 mmHg	76 mmHg	Mabey et al. 1982
Vapor density	8.7 (air=1)	No data	IARC 1991a, 1991b
Henry's law constant	5.6x10 ⁻⁴ atm-m ³ /mol	9.9x10 ⁻⁴ atm-m ³ /mol	Mabey et al. 1982
Surface tension	41.53 dynes/cm	No data	Lewis 1997
Heat of vaporization	46.05 KJ/mol (25 °C)	No data	Lide 2000
Autoignition temperature	No data	No data	
Flashpoint	No data	No data	
Flammability limits	Non-flammable	Non-flammable	HSDB 2004a, 2004b
Conversion factor	1 ppm = 10.34 mg/m ³ 1 mg/m ³ = 0.097 ppm	1 ppm = 8.52 mg/m ³ 1 mg/m ³ = 0.12 ppm	IARC 1999a, 1999b