

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

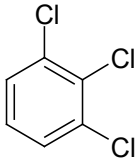
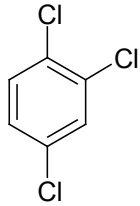
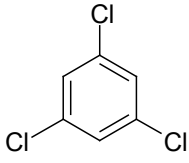
There are three possible isomers for trichlorobenzene: 1,2,3-trichlorobenzene; 1,2,4-trichlorobenzene; and 1,3,5-trichlorobenzene. The chemical identity of each isomer is shown in Table 4-1.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Trichlorobenzenes are relatively volatile, hydrophobic substances. The physical and chemical properties of each isomer are shown in Table 4-2.

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**Table 4-1. Chemical Identity of Trichlorobenzenes<sup>a</sup>**

Characteristic	1,2,3-Trichlorobenzene	1,2,4-Trichlorobenzene	1,3,5-Trichlorobenzene
Synonym(s)	Benzene, 1,2,3-trichloro-; vic-trichlorobenzene; AI3-15516	Benzene, 1,2,4-trichloro-; unsym-Trichlorobenzene; AI3-07775; 1,2,4-Triclorobenceno (Spanish)	Benzene, 1,3,5-trichloro-; s-Trichlorobenzene; sym-Trichlorobenzene
Chemical formula	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>
Chemical structure			
Identification numbers:			
CAS registry	87-61-6	120-82-1	108-70-3
RTECS	No data	DC2100000 <sup>b</sup>	No data
EPA hazardous waste	No data	No data	No data
EPA/OPP pesticide Code	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	No data
HSDB	1502	1105	132
EINECS	No data	204-428-0 <sup>c</sup>	No data
NCI	No data	No data	No data

<sup>a</sup>All information from HSDB 2010, unless otherwise noted.

<sup>b</sup>NIOSH 1994.

<sup>c</sup>European Communities 2003.

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**Table 4-2. Physical and Chemical Properties of Trichlorobenzenes<sup>a</sup>**

Property	1,2,3-Trichlorobenzene	1,2,4-Trichlorobenzene	1,3,5-Trichlorobenzene
Molecular weight	181.45	181.45	181.45
Physical description	Platelets from alcohol	Colorless liquid	White crystals
Melting point	51.3°C	16.92°C	62.8°C
Boiling point	218.5°C	213.5°C	208°C
Density	1.4533 g/cm <sup>3</sup> at 25°C	1.459 g/cm <sup>3</sup> at 20°C	1.456 g/cm <sup>3</sup> at 20°C
Odor	No data	Aromatic odor	No data
Solubility:			
Water	18 mg/L at 25°C	49 mg/L at 25°C	6.01 mg/L at 25°C
Organic solvent(s)	Slightly soluble in ethanol; very soluble in ether and benzene. Freely soluble in carbon disulfide	Sparingly soluble in alcohol; miscible with ether, benzene, petroleum ether, carbon disulfide	Sparingly soluble in alcohol; freely soluble in ether, benzene, petroleum ether, carbon disulfide, glacial acetic acid
Partition coefficients:			
Log K <sub>ow</sub>	4.05	4.02	4.19
Log K <sub>oc</sub>	3.21–3.90	3.10–4.03	2.80–3.82
Henry's Law constant	1.25x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	1.42x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	1.89x10 <sup>-3</sup> atm-m <sup>3</sup> /mol
Vapor pressure	0.21 mm Hg at 25°C	0.46 mm Hg at 25°C	0.24 mm Hg at 25°C
Autoignition temperature	No data	571°C	No data
Flashpoint	112.7°C	105°C	107°C
Flammability limits in air	No data	Lower flammable limit: 2.5% by volume at 302°F (150°C). Upper flammable limit: 6.6% by volume at 302°F (150°C)	No data
Conversion factors <sup>b</sup>	1 mg/m <sup>3</sup> =0.13 ppm	1 mg/m <sup>3</sup> =0.13 ppm	1 mg/m <sup>3</sup> =0.13 ppm
Explosive limits	No data	2.5–6.6 % volume (at 150°C)	No data

<sup>a</sup>All information from HSDB 2010, unless otherwise noted.<sup>b</sup>Verschueren 2001.