

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

Table 3-1 lists common synonyms, trade names, and other pertinent identification information for HMX.

#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

Table 3-2 lists important physical and chemical properties of HMX.

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**TABLE 3-1. Chemical Identity of HMX**

Characteristic	Information	Reference
Chemical name	HMX	
Synonym(s)	1,3,5,7-Tetranitro- 1,3,5,7-tetraazocyclooctane; cyclotetramethylenetrinitramine; tetramethylenetrinitramine; octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocene; octogen; and others	HSDB 1995; IRIS 1995
Registered trade name(s)	No data	
Chemical formula	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	HSDB 1995
Chemical structure	$  \begin{array}{c}  \text{NO}_2 \\    \\  \text{CH}_2 - \text{N} - \text{CH}_2 \\    \qquad \quad   \\  \text{O}_2\text{N}-\text{N} \qquad \quad \text{N}-\text{NO}_2 \\    \qquad \quad   \\  \text{CH}_2 - \text{N} - \text{CH}_2 \\    \\  \text{NO}_2  \end{array}  $	Bongiovanni et al. 1984
Identification numbers:		
CAS registry	2691-41-0	HSDB 1995
NIOSH RTECS	XF 7450000	HSDB 1995
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	UN0226	HSDB 1995
HSDB	5893	HSDB 1995
NCI	No data	

CAS = Chemical Abstracts Services; 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 3-2. Physical and Chemical Properties of HMX**

Property	Information	Reference
Molecular weight	296.20	HSDB 1995
Color	Colorless	EPA 1988
Physical state	Solid	EPA 1988
Melting point	276–286°C	Army 1989; EPA 1988
Boiling point	No data	
Density:		
at 25°C	1.90 g/cm <sup>3</sup>	Army 1989
Odor	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 20°C	6.63 mg/L	EPA 1988
Water at 25°C	5 mg/L	Army 1989
Water at 83°C	140 mg/L	EPA 1988
Organic solvent(s)	Soluble in dimethyl sulfoxide, acetone, cyclohexanone, acetic anhydride	EPA 1988
Partition coefficients:		
Log K <sub>ow</sub>	0.26; 0.06	Army 1989
Log K <sub>oc</sub>	0.54	Army 1989
Vapor pressure at 25°C	3.33x10 <sup>-14</sup> mmHg	Army 1989
at 100°C	3x10 <sup>9</sup> mmHg	EPA 1988
Henry's law constant:		
at 25°C	2.60x10 <sup>-15</sup> atm-m <sup>3</sup> /mol	Army 1989
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors	No data	
Explosive limits	Decomposes violently at 279°C	Sax and Lewis 1989

