

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; cycloctetramethylenetetranitramine; tetramethylenetetranitramine; octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine; octogen; and others | HSDB 1995; IRIS 1995 |
| Registered trade name(s) | No data | |
| Chemical formula | $C_4H_8N_8O_8$ | HSDB 1995 |
| Chemical structure | | 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 ³ | 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 _{ow} | 0.26; 0.06 | Army 1989 |
| Log K _{oc} | 0.54 | Army 1989 |
| Vapor pressure at 25°C | 3.33x10 ⁻¹⁴ mmHg | Army 1989 |
| at 100°C | 3x10 ⁻⁹ mmHg | EPA 1988 |
| Henry's law constant: at 25°C | 2.60x10 ⁻¹⁵ atm-m ³ /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 |

