

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 1-bromopropane is provided in Table 4-1.

Commercial 1-bromopropane has been reported to be 99% pure (ACGIH 2014). 1-Bromopropane used as a commercial solvent blend is formulated to improve performance and inhibit decomposition, including stabilization to prevent hydrolysis (NTP 2011) and is between 85 and 99% pure (UNEP 2001).

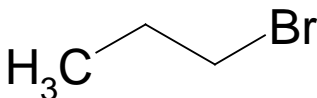
2-Bromopropane is present as a contaminant at 0.1–0.2% (OSHA 1999).

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1-bromopropane is provided in Table 4-2.

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

| Characteristic           | Information   |
|--------------------------|---|
| Chemical name            | 1-Bromopropane  |
| Synonym(s)               | Propane, 1-bromo-; propyl bromide; n-propyl bromide; 1-BP                         |
| Registered trade name(s) | Abzol; Ensolv; Solvon; Ensolv-NDI; Whisper Spray; Soft Seam <sup>b</sup>          |
| Chemical formula         | C <sub>3</sub> H <sub>7</sub> Br  |
| Chemical structure       |  |
| Identification numbers:  |   |
| CAS Registry             | 106-94-5  |
| NIOSH RTECS              | TX4110000 <sup>c</sup>  |
| EPA Hazardous Waste      | No data   |
| OHM/TADS                 | No data   |
| DOT/UN/NA/IMDG           | UN 2344; IMO 3  |
| HSDB                     | 1068  |
| NCI                      | No data   |

<sup>a</sup>All information obtained from HSDB (2013), unless otherwise noted.

<sup>b</sup>EPA 2007c.

<sup>c</sup>RTECS 2009.

CAS = Chemical Abstracts Services; CIS = Chemical Information System; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance 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 1-Bromopropane<sup>a</sup>**

| Property                            |   |
|-------------------------------------|---|
| Molecular weight (g/mol)            | 122.99  |
| Color                               | Colorless   |
| Physical state                      | Liquid  |
| Melting point                       | -110°C  |
| Boiling point                       | 71°C  |
| Density:<br>at 20°C/20°C            | 1.353   |
| Odor                                | Sweet   |
| Odor threshold:                     |   |
| Water                               | No data   |
| Air                                 | No data   |
| Taste                               | No data   |
| Solubility:                         |   |
| Water at 20°C                       | 2.45x10 <sup>3</sup> mg/L   |
| Other solvents                      | Soluble in acetone, ethanol, ether, benzene, chloroform, carbon tetrachloride |
| Partition coefficients:             |   |
| Log K <sub>ow</sub>                 | 2.10  |
| Log K <sub>oc</sub>                 | 40 (estimated)  |
| Vapor pressure at 20°C              | 110.8 mm Hg   |
| OH radical rate constant at 25°C    | 1.18x10 <sup>-12</sup> cm <sup>3</sup> /molecules-second <sup>b</sup>         |
| Henry's law constant at 20°C        | 7.3x10 <sup>-3</sup> atm-m <sup>3</sup> /mol (estimated)                      |
| Autoignition temperature            | 490°C   |
| Flashpoint                          | 21°C <sup>c</sup>   |
| Flammability limits at 25°C         | No data   |
| Incompatibilities                   | Strong oxidants; strong bases   |
| Conversion factors (25°C and 1 atm) | 1 mg/L=198.8 ppm; 1 ppm=5.03 mg/m <sup>3</sup>                                |
| Explosive limits                    | LEL=4.6%  |

<sup>a</sup>All information obtained from HSDB (2013), unless otherwise noted.

<sup>b</sup>Donaghy et al. (1993)

<sup>c</sup>Alfa Aesar (2014)