

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

The chemical formula, structure, synonyms, and identification numbers for trichloroethylene are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of trichloroethylene are listed in Table 3-2.

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TABLE 3-1. Chemical Identity of Trichloroethylene

| Characteristic | Information | Reference |
|--------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| Chemical name | Trichloroethylene | |
| Synonym(s) | Acetylene trichloride; 1-chloro-2,2-dichloroethylene; 1,1-dichloro-2-chloroethylene; ethylene trichloride; trichlororide; TCE; 1,1,2-trichloroethylene; trichloroethene | IARC 1979 |
| Registered trade name(s) | Algylen; Anamenth; Benzinol; Blacosolv; Blancosolv; Cecolene; Chlorilen; Chlorylea; Chlorylen; Chorylen; Cicosolv; Crawhaspol; Densinfluat; Dow-Tri; Dukeron; Fleck-Flip; Flock Flip; Fluate; Gumalgene; Germalgene; HI-TRI; Lanadin; Lethurin; Narcogen; Narkogen; Narkosoid; NEU-TRI; Nialk; Perma-A-Chlor; Perma-A-Clor; Petzinol; Philex; Threthylen; Threthylene; Tretylene; Triad; Trial; Triasol; Trichloran; Trichloren; Triclene; Tri-Clene; Trielene; Trielin; Triklone; Trilen; Trilene; Triline; Trimar; Triol; TRI-plus; TRI-plus M; Vestrol; Vitran; Westrosol | IARC 1979 |
| Chemical formula | C_2HCl_3 | SANSS 1990 |
| Chemical structure | $ \begin{array}{c} H \quad Cl \\ \backslash \quad / \\ C = C \\ / \quad \backslash \\ Cl \quad Cl \end{array} $ | |
| Identification numbers: | | |
| CAS registry | 79-01-6 | SANSS 1990 |
| NIOSH RTECS | KX4550000 | SANSS 1990 |
| EPA hazardous waste | U228 | HSDB 1994 |
| OHM/TADS | 7216931 | HSDB 1994 |
| DOT/UN/NA/IMCO shipping | UN1710 | HSDB 1994 |
| HSDB | 133 | HSDB 1994 |
| NCI | NCI-C04546 | HSDB 1994 |

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TABLE 3-1 (continued)

| Characteristic | Information | Reference |
|----------------|-------------|-----------|
|----------------|-------------|-----------|

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 Chemicals Substances

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TABLE 3-2. Physical and Chemical Identity of Trichloroethylene

| Property | Information | Reference |
|---------------------------------------------------------------------|-------------------------------------------------------------------------------------|--------------------------------|
| Molecular weight | 131.40 | HSDB 1994 |
| Color | Clear, colorless | HSDB 1994 |
| Physical state | Liquid (at room temperature) | HSDB 1994 |
| Melting point | -87.1°C | McNeill 1979 |
| Boiling point | 86.7°C | McNeill 1979 |
| Density: at 20°C | 1.465 g/mL | McNeill 1979 |
| Odor | Ethereal; chloroform-like; sweet | HSDB 1994 |
| Odor threshold: | | |
| Water | No data | |
| Air | 100 ppm | HSDB 1994 |
| Solubility: | | |
| Water at 20°C | 1.070 g/L | McNeill 1979 |
| at 25°C | 1.366 g/L | Tewari et al. 1982 |
| Organic solvent(s) | Miscible with many common organic solvents (such as ether, alcohol, and chloroform) | McNeill 1979; Windholz 1983 |
| Partition coefficients: | | |
| Log K_{ow} | 2.42 | Hansch and Leo 1985 |
| Log K_{oc} | 2.03–2.66 | Garbarini and Lion 1986 |
| Vapor pressure at 25°C | 74 mmHg | Mackay and Shiu 1981 |
| Henry's law constant: | | |
| at 20°C | 0.020 atm·m ³ /mol | Mackay and Shiu 1981 |
| at 25°C | 0.011 atm·m ³ /mol | Hine and Mookerjee 1975 |
| Autoignition temperature | None | McNeill 1979 |
| Flashpoint | None | McNeill 1979 |
| Flammability limits at 25°C (explosive limits) (volume % in air) | 8.0–10.5 | McNeill 1979 |
| Conversion factors | | Verschueren 1983 |
| Air at 20°C | 1 mg/m ³ = 0.18 ppm; 1 ppm = 5.46 mg/m ³ | |
| Water | 1 ppm (weight per volume) = 1 mg/L | |
| Explosive limits | No data | |