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Groundwater Chemicals Desk Reference

VOLUME 2

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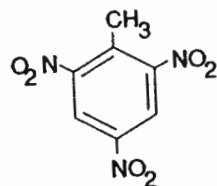


3634

2,4,6-TRINITROTOLUENE

Synonyms: Entsufo; 1-Methyl-2,4,6-trinitrobenzene; 2-Methyl-1,3,5-trinitrobenzene; NCI-C56155; TNT; α -TNT; TNT-tolite; Tolit; Tolite; Trilit; Trinitrotoluene; *sym*-Trinitrotoluene; Trinitrotoluol; α -Trinitrotoluol; *sym*-Trinitrotoluol; Tritol; Triton; Trotyl; Trotyl oil; UN 0209.

Structural Formula:



CHEMICAL DESIGNATIONS

CAS Registry Number: 118-96-7

DOT Designation: 1356

Empirical Formula: $C_7H_5N_3O_6$

Formula Weight: 227.13

RTECS Number: XU 0175000

PHYSICAL AND CHEMICAL PROPERTIES

Appearance: Colorless to light yellow monoclinic crystals.

Boiling Point: Explodes at 240 °C [1].

Log K_{oc} : 2.48 using method of Kenaga and Goring [2].

Log K_{ow} : 2.25 using method of Kenaga and Goring [2].

Melting Point: 82 °C [1]; 80.1 °C [3].

Solubility in Organics: Soluble in acetone, benzene, ether, and pyrimidine [1].

Solubility in Water: 0.013 wt % at 20 °C [4]; 1.42 g/L at 100 °C [3]; 200 mg/L at 15 °C [5].

2,4,6-Trinitrotoluene 833

Specific Density: 1.654 at 20/4 °C [1].

Transformation Products: 4-Amino-2,6-dinitrotoluene and 2-amino-4,6-dinitrotoluene, detected in contaminated ground-water beneath the Hawthorne Naval Ammunition Depot, NV., were reported to have formed from the microbial degradation of 2,4,6-trinitrotoluene [6].

Vapor Pressure: 0.05 mm at 85 °C [4]; 4.26×10^{-3} mm at 54.8 °C, 2.557×10^{-3} mm at 72.5 °C, 4.347×10^{-3} mm at 76.1 °C [7].

FIRE HAZARDS

Flash Point: Explodes [4].

HEALTH HAZARD DATA

Immediately Dangerous to Life or Health (IDLH): Not applicable [4].

Permissible Exposure Limits (PEL) in Air: 1.5 mg/m³ [8]; 0.5 mg/m³ [9].

MANUFACTURING

Selected Manufacturers: ChemService, Inc., P.O. Box 3108, 660 Tower Lane, West Chester, PA 19381-3108; Fisher Scientific Co., 711 Forbes Ave., Pittsburgh, PA 15219; Kodak Laboratory & Specialty Chemicals, Eastman Kodak Co., Rochester, NY 14650.

Uses: High explosive; intermediate in dyestuffs and photographic chemicals.

REFERENCES

1. Weast, R.C., Ed. *CRC Handbook of Chemistry and Physics*, 67th ed. (Boca Raton, FL: CRC Press, Inc., 1986), 2406 p.
2. Kenaga, E.E., and C.A.I. Goring. "Relationship between Water Solubility, Soil Sorption, Octanol-Water Partitioning and Concentration of Chemicals in Biota," in *Aquatic Toxicology, ASTM STP 707*, Eaton, J.G., Parrish, P.R., and A.C. Hendricks, Eds. (Philadelphia, PA: American Society for Testing and Materials, 1981), 115-122.