

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of guthion is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Guthion is a nonsystemic organophosphate insecticide. Pure guthion is a colorless to white, odorless, crystalline solid with a melting point range of 72–74 °C, while the technical-grade material is a cream to yellow-brown, granular solid with a melting point of 67–70 °C (EPA 2001b). Guthion is readily soluble in most organic solvents (acetone, toluene, chloroform, acetonitrile, benzene, xylene, carbon tetrachloride, and chlorobenzene), slightly soluble in methanol, ethanol, and propanol, and poorly soluble in water.

Information regarding the physical and chemical properties of this compound is located in Table 4-2.

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Table 4-1. Chemical Identity of Guthion

Characteristics	Guthion	References
Chemical name	S-(3,4-Dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-yl-methyl)O,O-dimethylphosphorodithioate	Tomlin 2003
Synonyms	O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)-methyl]	Tomlin 2003
Trade names	Guthion; Aziflo; Azin-PB; Crysthyon; Mezyl; Sniper; Supervalex	Tomlin 2003
Chemical formula	C ₁₀ H ₁₂ N ₃ O ₃ PS ₂	Tomlin 2003
Chemical structure	<p>The chemical structure shows a benzotriazine ring system. At the 3-position, there is a nitrogen atom bonded to a methyl group and a phosphorus atom. The phosphorus atom is part of a dimethylphosphorodithioate group, which consists of a central phosphorus atom double-bonded to a sulfur atom and single-bonded to two methoxy groups (OCH₃). The sulfur atom is also single-bonded to the phosphorus atom.</p>	Tomlin 2003
Identification numbers:		
CAS registry	86-50-0	Tomlin 2003
NIOSH RTECS	TE1925000	NIOSH 2005
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	NA 2783; Guthion mixture, liquid	HSDB 2006
HSDB	1171	HSDB 2006
NCI	No data	

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Table 4-2. Physical and Chemical Properties of Guthion

Property	Information	References
Molecular weight	317.3	Tomlin 2003
Color	Colorless to white (pure material); cream to yellow brown (technical grade material)	EPA 2001b
Physical state	Crystalline	Tomlin 2003
Melting point	72–74 °C (pure material); 67–70 °C (technical-grade material)	EPA 2001b
Boiling point	Decomposes above 200 °C	Tomlin 2003
Specific gravity (20 °C)	1.518	Tomlin 2003
Odor	Odorless	EPA 2001b
Odor threshold		
Water	0.0002 mg/kg	Verschueren 2001
Air	No data	
Solubility		
Water at 25 °C	28 mg/L	Tomlin 2003
Organic solvents	>250 g/L in dichloroethane, acetone, acetonitrile, ethyl acetate, and DMSO; 1.2 g/L in n-heptane and 170 g/L in xylene (all at 20 °C)	Tomlin 2003
Partition coefficients		
Log K_{ow}	2.75	Hansch et al. 1995
Log K_{oc}	2.69–3.67	Gawlik et al. 1998
Vapor pressure		
20 °C	3×10^{-5} Pa (2.2×10^{-7} mm Hg)	Suntio et al. 1988
Henry's law constant	3.7×10^{-9} atm·m ³ /mol	EPA 1999a
Flashpoint (closed cup)	No data	
Flammability limits		
Air	No data	
Conversion factors ^a		
ppm (v/v to mg/m ³ in air (20 °C))	1 ppm = 13.2 mg/m ³	Verschueren 2001
mg/m ³ to ppm (v/v) in air (20 °C)	1 mg/m ³ = 0.076 ppm	Verschueren 2001
Explosive limits	No data	

^aGuthion exists partially in the particulate-phase in the atmosphere. This conversion is only applicable to vapor-phase guthion.