## Section 2

## CHEMISTRY ASSESSMENT

# 1. ACTIVE CONSTITUENT

## 1.1 Chemical Identity

Chlorfenvinphos is an organophosphorus insecticide and acaricide used in the control of flies, fleas, mites and moths in and around agricultural buildings, pastures, and potato crops. Chlorfenvinphos is also widely used in external paraciticide formulations for use on cattle, sheep, deer, goats, horses and dogs. Technical chlorfenvinphos (comprised of the sum of E- and Z-isomers) has a minimum purity of 900 g/L. Typically, the ratio of isomers ZE is 8.6:1 in the technical material, with both the cis and the trans isomers having insecticidal activity. Whilst the potency of the isomers varies from species to species, the trans isomer is usually the more active one.

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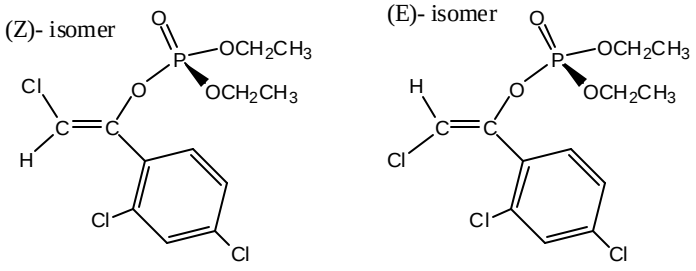
|---|---|
| Common name: | Chlorfenvinphos |
| IUPAC Name: | 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate |
| CA Name: | 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate |
| CAS Registry Numbers: | |
| (Z)- and (E)- isomers | 2701-86-2 |
| (Z)- isomer | 18708-87-7 |
| (E)- isomer | 18708-86-6 |
| Empirical Formula: | $C_{12}H_{14}Cl_3O_4P$ |
| Molecular weight: | 359.57 |
| Manufacturers' code no.: | SD 7859; C 8949 (Ciba-Geigy)<br>GC 4072 (Allied); CGA 26351<br>ENOLOFOS®; OMS 166; OMS 1328; ENT 24 969 |
| Synonyms: | "Birlane", "Supona", CL 58,085; SD 7859; GLC 4072 |
| Structural formula: | |



## 1.2 Physical and Chemical Properties

### *1.2.1 Physical and chemical properties of the pure active constituent and the TGAC*

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|---|---|
| Colour | pure active - clear, colourless<br>TGAC – amber to brown |
| Odour | mild specific odour |
| Physical State | liquid at 25 $^{o}$C |
| Melting point | -23 to –19 $^{o}$C |
| Boiling point | 167 to 170 $^{o}$C (at 0.5 mm Hg)<br>110 $^{o}$C (at 0.001 mm Hg) |
| Octanol/water partition coefficient (log P) | |
| (Z)- and (E)- isomers | 3.85 |
| (Z)- isomer | 4.22 |
| (E)- isomer | 3.81 |
| Specific gravity/density | 1.36 at 15/20 $^{o}$C |
| Refractive Index | 1.5272 ($N_D^{25}$) |
| Vapour pressure (volatility) | 2.2 x $10^{-7}$ mbar at 25 $^{o}$C |
| Water solubility (at 23 $^{o}$C) | 145 mg/L (at 23 $^{o}$C) |
| Solvent solubility | Miscible with most common organic solvents e.g. ethanol, acetone, dichloromethane, hexane, xylem, propylene, glycol, and kerosene |
| pH Stability | Hydrolysed slowly in neutral, acidic and slightly alkaline aqueous solutions; Hydrolysed rapidly in strongly alkaline solutions. |
| Thermal stability | Extremely stable at high temperature. Rapid decomposition only at temperatures above 150 $^{o}$C. Non-flammable. |
| Hydrolysis | Decomposes very slowly in water with $t_{½}$ >400 hours (pH 9.1, temp 38 $^{o}$C), and at pH 1.1, $t_{½}$ >700 hours.<br>Hydrolysis half-life in water at 20-30 $^{o}$C:<br>pH 3-5, $t_{½}$ = 200 days<br>pH 6, $t_{½}$ = 170 days<br>pH 9, $t_{½}$ = 80 days<br>pH 11, $t_{½}$ = 5 days |
| Henry's Law (K):<br>(various sources) | 1.55 X $10^{-3}$ Pa.m$^3$/mol<br>2.5 X $10^{-3}$ Pa.m$^3$/mol at 20$^{o}$C<br>2.80 X $10^{-4}$ Pa.m$^3$/mol |

## 1.3 Comments on Physio-chemical Properties

The vapour pressure and Henry's Law Constant indicate that chlorfenvinphos has a low volatility and is unlikely to volatilise from water or moist soil surfaces. It is moderately to very soluble in water at common environmental temperature ranges. The log $K_{ow}$ shows a moderate bioconcentration potential in aquatic

organisms. The Mackay level 1 fagacity model predicts 55% partitioning into water with 22% in soil, 20% in sediment and 2% in air at equilibrium (US EPA 1998) using a vapour pressure of 2.95 X $10^{-2}$ Pa and Henry's Law constant of 1.13 X $10^{-1}$ Pa.$m^3$/mol which indicate greater volatility.

### 1.4 Chemistry Aspects

The chemistry aspects (manufacturing process, quality control procedures, batch analysis results, and analytical methods) of chlorfenvinphos TGAC were evaluated and found acceptable. The chlorfenvinphos content of the TGAC is determined by GLC with flame ionisation detection.

## 2. FORMULATION OF THE END-USE PRODUCT

Registered uses for chlorfenvinphos include both agricultural applications (ie emulsifiable concentrate formulations used on agricultural/farm buildings, lucerne pasture, mushroom casing, and potato crops) and animal treatments (ie topical aerosol sprays, wound dressings, and dip and jetting liquids used to kill external parasites on cattle, sheep, horses, deer, goats and dogs). The mode of chlorfenvinphos action is non-systemic, and exposure of insects, mites and flies to the active (via contact and/or ingestion) affects the nervous system by inhibiting the activity of acetyl cholinesterase.

## 3. DECLARATION OF COMPOSITION

The Australian minimum compositional standard for chlorfenvinphos TGAC requires that the sum of the isomers (Z and E) comprise not less than 900 g/L of the technical material. The NRA-approved source of technical chlorfenvinphos meets this standard. All impurities that are present in the chlorfenvinphos TGAC at concentrations of 1 g/L or more are listed in the DoC.

There is no FAO monograph specification for technical chlorfenvinphos.

### 3.1 Toxic Impurities

The toxicologically significant compounds (sulfotepp, N-nitrosamines, halogenated dibenzo-pi-dioxins, halogenated dibenzofurans and PCBs) are not expected to occur in the chlorfenvinphos TGAC, due to the raw materials and synthetic route used in the manufacture of the material.

## 4. CONCLUSION

The NRA minimum compositional standard for chlorfenvinphos TGAC requires that the sum of the isomers (Z and E) comprise not less than 900 g/L of the technical material. This standard is to be retained.