

IUPAC Project Progress Report

Project number: 2003-011-3-600

Project Title: A critical compendium of pesticide physical chemistry data

Task Group Leaders: Wauchoper/Shaw

Report:

No formal project report was received. Nevertheless the project seems to progress well. The following text is an extract from the minutes of a Joint Meeting between IUPAC Project "Global Availability of Information on Agrochemicals", IUPAC Project "A Critical Compendium of Pesticide Physical Chemistry Data" and the FAO/IAEA INFOCRIS (International Food Contaminant and Residue Information System) held at the IAEA, Vienna, 18th September, 2004 (prepared by J.B. Unsworth)

"The IUPAC project A Critical Compendium Of Pesticide Physical Chemistry Data (the "Compendium" project) co-chaired by David Shaw and Don Wauchope. This project is designed to "establish an IUPAC compendium of critically evaluated values for aqueous solubility, vapour pressure, octanol/water partition coefficient (Kow) and acid/base dissociation constant (pKa) for active ingredients of pesticides", see <http://www.iupac.org/projects/2003/2003-011-3-600.html>. This project grew out of dissatisfaction with the quality of documentation, and sometimes the wide range of reported values for the fundamental physical/chemical properties of pesticide chemicals.

The "Compendium" project will be extended to include the parameters such as aqueous solubility, vapour pressure, octanol/water partition coefficient, acid/base dissociation constant, molecular weight, melting point, Henry's law constant, solubility in organic solvents (acetone, toluene, hexane)

The data from the project will be published in "journal" form which will be referenced by the INFOCRIS in the physicochemical properties Table as the authoritative critical evaluation/peer review.

A list of 60 has been proposed to give a good mix of old and new, plus being representative of various important pesticide families"