EPI Suite™–Estimation Program Interface

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What is EPI Suite ™?

The EPI (Estimation Programs Interface) Suite™ is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by EPA's and Syracuse Research Corp. (SRC).

EPI Suite™ uses a single input to run the following estimation programs: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, BioHCwin, KOCWIN™, WSKOWWIN™, WATERNT™, BCFBAF™, HYDROWIN™, KOAWIN and AEROWIN™, and the fate models WVOLWIN™, STPWIN™ and LEV3EPI™. ECOSAR™, which estimates ecotoxicity, is also included in EPI Suite™.

EPI Suite™ is a screening-level tool and should not be used if acceptable measured values are available.

A clear understanding of the estimation methods and their appropriate application is very important. Click on the Help tab in EPI Suite™ for detailed information on the methods and models in it.

How are EPI Suite™ estimates used?

EPI Suite™ provides users with estimates of physical/chemical and environmental fate properties.

Before using EPI Suite™, users should first determine whether any suitable data are available from the literature (e.g., Merck Index, Beilstein). This is facilitated by a database of >40,000 chemicals (called PHYSPROP©) that is included in the EPI Suite™ software. Dermwin™, a program that estimates the dermal permeability coefficient Kp, and is included in EPI Suite™. ECOSAR™ is a program that predicts aquatic toxicity and is included in EPI Suite™. ECOSAR™ can also be downloaded as a separate program from the ECOSAR home page.

Go to ECOSAR. <https://epa.gov/expobox>

Individual models in EPI Suite™

- KOWWIN™: Estimates the log octanol-water partition coefficient, log KOW, of chemicals using an atom/fragment contribution method.
- AOPWIN™: Estimates the gas-phase reaction rate for the reaction between the most prevalent atmospheric oxidant, hydroxyl radicals, and a chemical. Gas-phase ozone radical reaction rates are also estimated for olefins and acetylenes. In addition, AOPWIN™ informs the user if nitrate radical reaction will be important. Atmospheric half-lives for each chemical are automatically calculated using assumed average hydroxyl radical and ozone concentrations.
- HENRYWIN™: Calculates the Henry's Law constant (air/water partition coefficient) using both the group contribution and the bond contribution methods.

- MPBPWIN™: Melting point, boiling point, and vapor pressure of organic chemicals are estimated using a combination of techniques. Included is the subcooled liquid vapor pressure, which is the vapor pressure a solid would have if it were liquid at room temperature. It is important in fate modeling.
- BIOWIN™: Estimates aerobic and anaerobic biodegradability of organic chemicals using 7 different models. Two of these are the original Biodegradation Probability Program (BPP™). The seventh and newest model estimates anaerobic biodegradation potential.
- BioHCwin: Estimates biodegradation half-life for compounds containing only carbon and hydrogen (i.e. hydrocarbons).
- KOCWIN™: Formerly called PCKOCWIN™, this program estimates the organic carbon-normalized sorption coefficient for soil and sediment; i.e. KOC. KOC is estimated using two different models: the Sabljic molecular connectivity method with improved correction factors; and the traditional method based on log KOW.

And other models that make up EPI Suite:™

- WSKOWWIN™: Estimates an octanol-water partition coefficient using the KOWWIN™ program, then estimates a chemical's water solubility from this value and applicable correction factors if any.
- WATERNT™: Estimates water solubility directly using a "fragment constant" method similar to that used in the KOWWIN™ program.
- BCFBAF™: Formerly called BCFWIN™, this program estimates fish bioconcentration factor and its logarithm using two different methods. The first is the traditional regression based on log KOW plus any applicable correction factors, and is analogous to the WSKOWWIN™ method. The second is the Arnot-Gobas method, which calculates BCF from mechanistic first principles. BCFBAF also incorporates prediction of apparent metabolism half-life in fish, and estimates BCF and BAF for three trophic levels.

- HYDROWIN™: Estimates aqueous hydrolysis rate constants and half-lives for the following chemical classes: esters, carbamates, epoxides, halomethanes, selected alkyl halides, and phosphorus esters. Estimates rate constants for acid- and base-catalyzed hydrolysis, but with the exception of phosphorus esters, not neutral hydrolysis. In addition, HYDROWIN™ identifies a variety of chemical structure classes for which hydrolysis may be significant (e.g. carbamates) and gives relevant experimental data.
- KOAWIN: Estimates KOA, the octanol/air partition coefficient, using the ratio of the octanol/water partition coefficient (KOW) from KOWWIN™ and the dimensionless Henry's Law constant (KAW) from HENRYWIN™. KOA has multiple uses in chemical assessment.
- AEROWIN™: Estimates the fraction of airborne substance sorbed to airborne particulates, i.e. the parameter phi (ϕ), using three different methods. AEROWIN™ results are also displayed with AOPWIN™ output as an aid in interpretation of the latter.
- WVOLWIN™: Estimates the rate of volatilization of a chemical from rivers and lakes; and calculates the half-life for these two processes from their rates. The model makes certain default assumptions with respect to water body depth, wind velocity, etc.

And more:

- STPWIN™: Using several outputs from EPI Suite™, this program predicts the removal of a chemical in a typical activated sludge-based sewage treatment plant. Values are given for total removal and three processes that may contribute to removal: biodegradation, sorption to sludge, and air stripping. The program assumes a standard system design and set of default operating conditions.
- LEV3EPI™: This program contains a level III multimedia fugacity model and predicts partitioning of chemicals among air, soil, sediment, and water under steady state conditions for a default model "environment". Some (but not all) system default values can be changed by the user.

- ECOSAR™ Version 1.11 (Sept 2012): The Ecological Structure Activity Relationships (ECOSAR) Class Program estimates the aquatic toxicity of industrial chemicals. The program estimates acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms to fish, aquatic invertebrates, and green algae, and has limited SARs for other salt water and terrestrial species, where data were available. This program is maintained by a separate division in the Agency and more information on the model can be found on the ECOSAR webpage.

Go to ECOSAR. <https://epa.gov/expobox>

Peer review of EPI Suite™

Individual estimation programs and/or their underlying predictive methods and equations have been described in numerous journal articles in peer-reviewed technical journals. The full reference citations are given in the Help files for the individual programs.

In addition, EPI Suite™ has undergone detailed review by a panel of EPA's independent Science Advisory Board (SAB). The 2007 report can be found on the SAB Advisory Reports page.

Citing EPI Suite™

Full reference citations for the individual programs are given in the Help files for the individual programs. Cite the software itself as follows:

US EPA. [2012 or insert current year]. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11 or insert version used]. United States Environmental Protection Agency, Washington, DC, USA.

Hardware and software requirements?

EPI Suite™ v4.11 runs on Windows NT®, Windows XP/XP Professional®, and Windows Vista®, and Windows 7. All of the individual programs and help files also work correctly on Windows 95® and 98® when opened from within the EPI Suite™ folder, but users of

the interface program may encounter error messages.

Users of Windows Vista: please see the special instructions on the download page.

Download and install EPI Suite™

Download EPI Suite™ 4.11 <https://epa.gov/tsca-screening-tools/download-epi-suitetm-estimation-program-interface-v411>

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