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# ***Predicting Chemical Properties and Fate Using the Estimation Programs Interface (EPI) Suite™ of Models***

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**International Science Forum on Computational  
Toxicology, RTP, North Carolina**

**23 May 2007**

**U.S. Environmental Protection Agency  
Office of Pollution Prevention and Toxics  
Washington, DC 20460**



# Office of Prevention, Pesticides, and Toxic Substances

- Develops national strategies for toxic substances control and promotes pollution prevention and the public's right to know about chemical risk
- Office of Pesticide Programs (OPP)
- Office of Pollution Prevention and Toxics (OPPT)
- Office of Science Coordination and Policy (OSCP)

# Office of Pollution Prevention and Toxics

- Pre-manufacture review of new industrial chemicals
- Testing, assessment, and risk reduction of existing industrial chemicals
- Management of “national chemicals” (e.g. PCBs)
- International chemical issues (e.g. POPs)
- Pollution prevention advocacy
- Partnership programs, e.g. HPVC Challenge, Green Suppliers Network, DfE and Green Chemistry



# Estimation Programs Interface (EPI Suite™)

- Estimates physical/chemical properties and environmental fate and transport
- Runs estimation programs sequentially with chemical structure as only input
- Includes PHYSPROP, a database of measured properties for >40,000 chemicals
- Considered a screening-level tool; not applicable to all substances
- Intended for use only in absence of measured values

# *Things to Look for in Estimation Software*

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- (1)** How comprehensive is the methodology?
- (2)** How accurate are the methods?
- (3)** Have the methods been validated?
- (4)** Have the methods been published / peer-reviewed?
- (5)** Is the software easy to use?
- (6)** Does it
  - (a)** Run structures batchwise?
  - (b)** Provide adequate help information?



# Chemical Property and Fate Programs in EPI Suite™



## P/Chem Property Programs

<b>AEROWIN</b>	sorption to atmospheric particulates ( $\phi$ )
<b>BCFWIN</b>	bioconcentration factor
<b>HENRYWIN</b>	Henry's law constant; air-water partition coefficient
<b>KOAWIN</b>	octanol-air partition coefficient
<b>KOWWIN</b>	octanol-water partition coefficient
<b>MPBPWIN</b>	melting point, boiling point, vapor pressure
<b>PCKOCWIN</b>	soil organic carbon sorption coefficient
<b>WSKOWWIN</b>	water solubility from log Kow
<b>WATERNT</b>	water solubility from fragments



# Chemical Property and Fate Programs in EPI Suite™



## Environmental Fate Programs

### *degradation processes*

<b>AOPWIN</b>	atmospheric oxidation
<b>BIOWIN</b>	biodegradability
<b>BioHCWIN</b>	biodegradability of hydrocarbons
<b>HYDROWIN</b>	aqueous hydrolysis

### *multimedia fate*

<b>STPWIN</b>	removal in activated sludge treatment
<b>LEVEL III</b>	transport/distribution by fugacity model
<b>WVOWIN</b>	volatilization from water

# A Brief History of EPI


- 1980
  - “Lyman” published—the original handbook of estimation methods—Lyman, Rheel and Rosenblatt
  - Hand calculators widely used
  - Only mainframe computers available
- Early 1980s
  - Personal computers become common in EPA offices, but not yet 1 for every person
  - Lyman methods encoded in a DOS program called “CHEMEST”
- About 1986
  - First fragment-based biodegradation models developed—now called BIOWIN1 &2



# A Brief History of EPI, cont.

- About 1990/1991
  - Sabljic's molecular connectivity-based Koc method enhanced and encoded in a DOS program
  - Atmospheric Oxidation Program (AOP) and Henry program (now HENRYWIN) developed
- Early 1990s
  - BLOWIN "expert survey" models developed—now called BLOWIN3 and 4
  - EPA asked, "Why not unite the growing collection of methods in a 'shell program' for easier use?"
  - The shell program is named EPI—the Estimation Programs Interface—and first appears in DOS format

## A Brief History of EPI, cont.

- Mid 1990s
    - More new models: MPBPWIN, KOWWIN, WSKOWWIN
    - SRC sees the future and converts EPI (DOS) on its own to EPIWIN
  - Late 1990s
    - BCFWIN; fugacity models (STP and EQC); more
  - 2000 to present
    - Many user interface and convenience features added. Several new models
    - EPIWIN copyright purchased by EPA. EPA renamed it EPI Suite and has ***sole ownership***
-  EPI Suite is a result of an ***evolutionary process***, not a grand plan

# EPI Suite™ Download Page

The screenshot shows a Mozilla Firefox browser window displaying the EPA/OPPT website. The address bar shows the URL: <http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm>. The page title is "EPA/OPPT/Exposure Assessment Tools and Models/Download EPI Suite v3.12 - Mozilla Firefox".

The main content area features the EPA logo and the heading "Exposure Assessment Tools and Models". Below this, there are links for "Recent Additions" and "Contact Us", and a search bar. The breadcrumb trail reads: "You are here: [EPA Home](#) > [Exposure Assessment Tools and Models](#) > [Estimation Programs Interface \(EPI\) Suite](#) > Download EPI Suite v3.20 (February, 2007)".

The primary heading is "Download EPI Suite v3.20". Below it, a "Copyright Notice; Terms and Conditions of Use:" section states: "© 2000 - 2007 U.S. Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN." It further explains that the software is owned by the EPA and that users are granted permission to download and use it on their personal and business computers, with certain restrictions on modification and redistribution.

A link for "Description of Updates for EPI Suite Version 3.20 (February, 2007)" is provided. Below this, a download link for "epi320.zip" (19.53MB) is shown with a green circular icon.

The "Download And Install Instructions" section provides the following steps:

1. Double click EPI320.zip.
2. Save EPI320 to a directory of your choice.
3. Execute the file named " Setup.exe" located in the directory that you chose and follow the instructions at each screen to proceed. By default, the EPISUITE software is installed in C:\EPISUITE and a shortcut icon is placed in the EPI Suite folder under Windows Start Menu.

The browser's taskbar at the bottom shows the Start button, several open applications (including Internet Explorer, a folder named "J:\Co...", and a file named "4 M..."), and the system tray with the time "10:12 AM".

# EPI Suite™ v3.20 Input Screen (Feb 2007)

**EPI v3.20** [ \_ [ ] [ X ]

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp Previous Get User Save User CAS Input CALCULATE ClearInputField What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m<sup>3</sup>/mole):  Wat Sol (mg/L):  MP:

Vap Pr (mm Hg):  BP:

Water Depth (meters): 

River:	1	Lake:	1
Wind Velocity (m/sec):	5		0.5
Current Velocity(m/sec):	1		0.05

 Log Kow:

Output  
 Summary  
 Full



The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

Important information on the performance, development and application of the individual estimation programs within EPI Suite™ is included in the User's Guide.

© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.

# EPI Suite™ Chemical Structure Entry

- Runs from SMILES representation of chemical structure
- SMILES can be entered directly or using a chemical's CAS number
- Chemicals can be run batchwise
- Accepts MDL Mol files (generated by Isis Base/Draw)

# EPI Suite™ Core Property Estimation Programs

- MPBPWIN
  - Estimates properties at 25 C; if run as a standalone, VP can be estimated for any temperature of interest
  - Various methods used, including Joback, Stein and Brown, Antoine, others
- KOWWIN
  - If run as a standalone, can provide an estimate using the “experimental value adjusted” (analog) method
- WSKOWWIN
- WATERNT
  - If run as a standalone, can provide an estimate using the “experimental value adjusted” method

# EPI Suite™ Property Estimation Programs, cont.

- HENRYWIN
  - Henry's Law constant from bond/group contribution methods (improved Hine-Mookerjee)
  - If run as a standalone, can estimate  $H_c$  as a function of temperature, and using the “experimental value adjusted” method
- BCFWIN
  - Metabolism not considered
- PCKOCWIN
  - Organic carbon partition coefficient from molecular connectivity

# EPI Suite™ Transformation (Degradation) Programs

- AOPWIN
  - Rate constants for hydroxyl radical and ozone oxidation in the atmosphere
- BIOWIN
  - Biodegradability using seven predictive models
  - Semi-quantitative rates from two models, likelihood of fast degradation from the other five
- HYDROWIN
  - Hydrolysis rate constants for acid- and base-catalyzed reactions, but only for a small number of classes
  - Neutral hydrolysis rate not estimated



# EPI Suite™ Modeling Programs

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## (1) Rate of volatilization from water

EPI adaptation of model from Lyman Handbook

**Results:** volatilization half-lives for model river & lake

## (2) Sewage treatment plant model

EPI adaptation of Mackay's Toronto (STP) Model

**Results:** percent removal (air, biodegradation, sludge)

## (3) Level III fugacity model

EPI adaptation of Mackay's EQC Model

**Results:** overall persistence; mass distribution in air, water, soil, sediment

# EPI Suite™: New Properties and Methods in v3.20

- Subcooled liquid vapor pressure—to MPBPWIN
- Air/water partition coefficient (dimensionless Henry constant,  $K_{AW}$ )—to HENRYWIN
- Octanol/air partition coefficient ( $K_{OA}$ )—new model KOAWIN
- Fraction of airborne substance in particulates ( $\phi$ ), by 3 methods—new model AEROWIN
- Methanogenic anaerobic biodegradation potential—to BIOWIN as “BIOWIN7”
- Biodegradation half-life of hydrocarbons—new model BioHCWIN

# EPI Suite™ v3.20 Input Screen (Feb 2007)

EPI v3.20

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp Previous Get User Save User CAS Input CALCULATE ClearInputField What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m<sup>3</sup>/mole):

Wat Sol (mg/L):

MP:

Vap Pr (mm Hg):

BP:

Water Depth (meters):

River:

Lake:

Wind Velocity (m/sec):

Current Velocity(m/sec):

Log Kow :

Output

Summary

Full



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© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.

EPI v3.20

What's New

File Edit Functions File Edit Bookmark Options Help

PhysProp Prev Contents Index Back Print

## What's New in EPI Suite v3.20

### Program Modifications & New Features in v3.20:

1. A new model has been added to the Biowin system of biodegradability prediction models. It is BioAnWin, which estimates anaerobic biodegradation potential
  - The model predicts fast/slow degradation in the "serum bottle" test, OECD 311
  - The test conditions are most relevant to anaerobic digesters. Anaerobic digestion is a treatment phase in almost every POTW
  - The model uses a BIOWIN fragment contribution approach
2. A new biodegradability model for hydrocarbons has been added: BioHCWin
  - BioHCWin estimates biodegradation half-life for compounds containing only carbon and hydrogen
  - The model uses a fragment contribution approach
  - Support for BioHCWin development was provided by CONCAWE
3. Subcooled liquid vapor pressure prediction has been added to MPBPVP. Subcooled liquid VP is the vapor pressure a solid would have if it were liquid at ambient temperature. It is the most relevant vapor pressure value for solids in environmental partitioning (e.g. in multimedia models, and is needed to estimate aerosol-particulate partitioning using the Junge-Pankow method
4. The Henrywin program now calculates and displays the dimensionless Henry constant or KAW, also known as the air/water partition coefficient
  - Needed to estimate octanol/air partition coefficient (KOA)
  - Other uses in prediction:
    - ... Volatilization from water
    - ... Plant uptake: water fraction of foliage
    - ... Rain and snow scavenging
5. A new program called Koawin has been added. The program estimates the octanol/air partition

Enter SMILES:

Chem NAME:


NameLookup

Henry LC (atm-m<sup>3</sup>/mol)

Water Depth (meters)

Wind Velocity (m/sec)

Current Velocity(m/sec)



Start B... 2 4 E... E... CH 2 W... 10:46 AM

# EPI Suite™: Method Details, Accuracy, Validation

- Method details
  - Estimation methods for chemical properties and degradation are based on standard regression techniques
  - Most use correction factors
  - Method details are summarized online in the Help files
  - Full reference citations are also given so that users can examine methods in more detail, if they desire





PhysProp Previous Get User Save User CAS Input CALCULATE

Enter SMILES:

Chem NAME:   
NameLookup

Henry LC (atm-m<sup>3</sup>/mole):  Wat Sol (mg/L):   
Vap Pr (mm Hg):

	River:	Lake:	Log Kow:
Water Depth (meters):	<input type="text" value="1"/>	<input type="text" value="1"/>	<input type="text"/>
Wind Velocity (m/sec):	<input type="text" value="3"/>	<input type="text" value="0.5"/>	
Current Velocity(m/sec):	<input type="text" value="1"/>	<input type="text" value="0.05"/>	

- EPI Suite User Guide
- SMILES Help
- What's New in EPI v3.20
- AEROWIN Help
- AOPWIN User Guide
- AOP Accuracy Doc
- BCFWIN User Guide
- BioHCwin User Guide**
- BIOWIN User Guide
- ECOSAR User Guide
- HENRYWIN User Guide
- HYDROWIN User Guide
- KOAWIN User Guide
- KOWWIN User Guide
- MPBPWIN User Guide
- PCKOCWIN User Guide
- WSKOWWIN User Guide
- WATERNT User Guide
- Fugacity Model Help
- STP Model Help
- Water Volatilization Model Help
- About EPI Suite...



The Estimation Programs Interface (EPI) Suite™ was developed by the United States Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. As a screening tool, it is intended for use in screening level applications such as to quickly screen for release potential, and "bin" chemicals by priority for future work. Estimated values are used when experimental (measured) values are available.

Important information on the performance, development and application of the estimation programs within EPI Suite™ is included in the User's Guide.

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EPI v3.20 BioHCwin

File Edit Function

File Edit Bookmark Options Help

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***On-Line BioHCwin User's Guide (v1.01)***

- [1.0. Introduction & Overview](#)
- [2.0. Computer Software Requirements](#)
- [3.0. Installed Files](#)
- [4.0. Starting BIOHCWIN](#)
- 5.0. Data Entry & Edit Keys
  - [5.1. Entering Data](#)
  - [5.2. Function Keys & Buttons](#)
  - [5.3. Importing Structures](#)
- 6. Methodology & Results
  - [6.0. Structure Window](#)
  - [6.1. Methodology of the BioHCwin Model](#)
- 7.0. Batch Runs
  - [7.1. Batch Output Formats](#)
- 8.0. Bibliography

[Appendix A - Selected SMILES Information](#)  
[Appendix B - Description of User Input File](#)  
[Appendix C - CAS Number Database](#)  
[Appendix D. Fragment Coefficients for the BioHCwin Model](#)  
[Appendix E - Chemicals Used to Derive the BioHCwin Model](#)  
[Appendix F - Structure Drawing Programs That Can Generate SMILES Notations](#)

For Help concerning SMILES Notations, go to the on-line help file containing ["A Brief Description of SMILES Notation"](#).

PhysProp

Enter SMILES:

Chem NAME:


NameLookup

Henry LC (atm-m)

Water Depth (m)

Wind Velocity (m)

Current Velocity(m)



Start Bob... J:\... 4 M... EPA... EPI... Bio... 10:16 AM

# EPI Suite™: Method Details, Accuracy, Validation

- Method details
- Accuracy
  - EPA considers the accuracy acceptable for a screening-level tool
  - Information on method error is summarized online in the Help files
  - Full reference citations are also given so that users can examine the statistics in more detail, if they desire



# KOWWIN Program - $\log K_{ow}$ ( $\log P$ )

## Methodology - Atom/Fragment

### Contributions:

170 Fragments

290 Correction Factors

### Log Kow used by:

BCFWIN

DERMWIN

ECOSAR

WSKOWWIN

### Statistical Accuracy:

	<u>number</u>	<u>Corr (<math>r^2</math>)</u>	<u>Std Dev</u>	<u>Mean Error</u>
Total	13229	0.954	0.436	0.316
Training	2467	0.981	0.219	0.162
Validation	10762	0.943	0.473	0.354

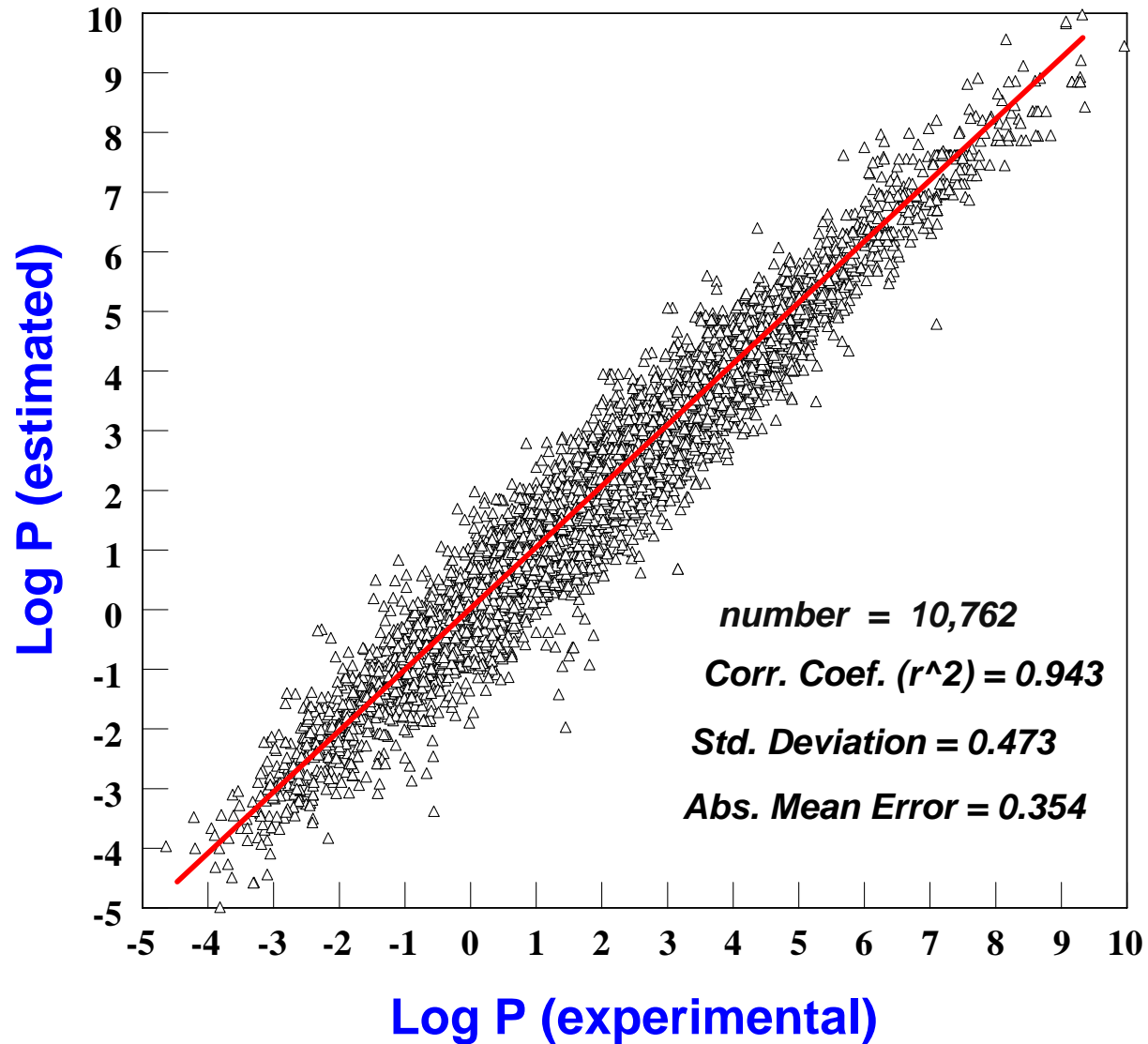
KOWWIN includes the experimental database of 13,229 recommended  $\log P$  values

**Journal Article Description: J. Pharm. Sci. 84(1): 83-92 (1995)**

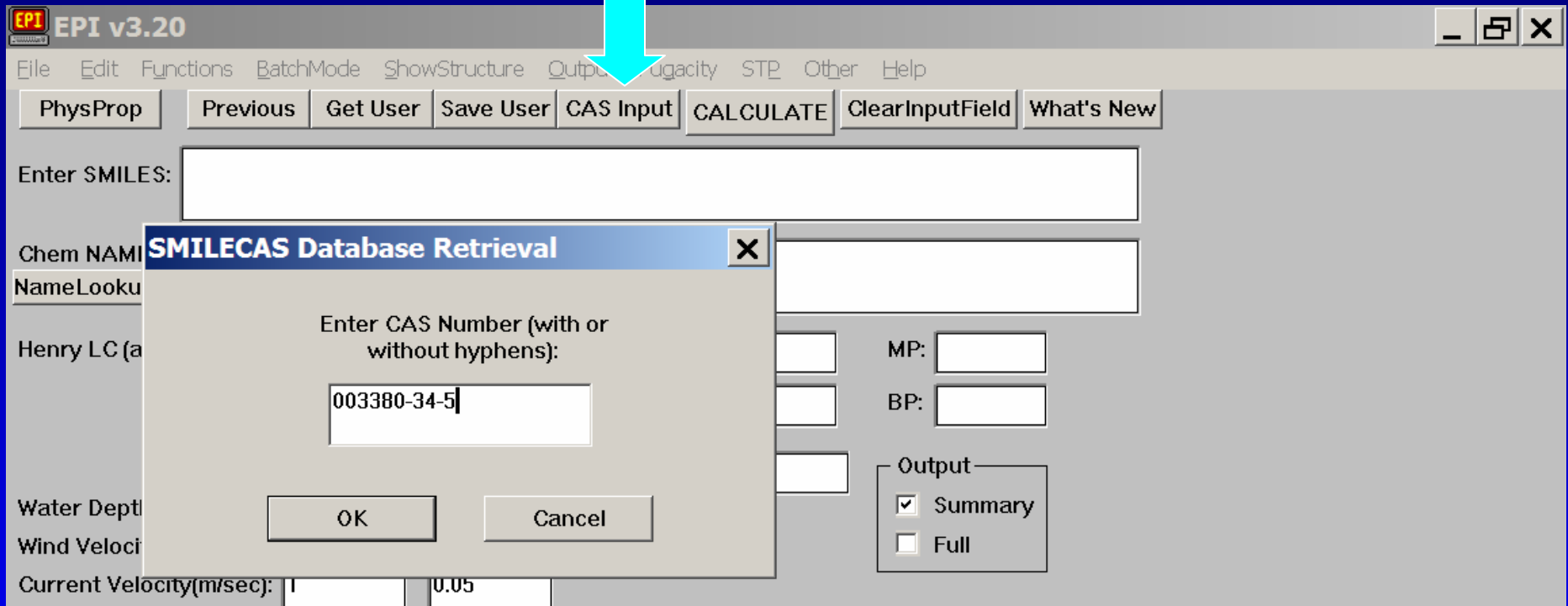
# EPI Suite™: Method Details, Accuracy, Validation

- Method details
- Accuracy
- Validation
  - Most methods have been validated using independent (external) validation sets
  - Information on validation is summarized online in the Help files
  - Full reference citations are also given so that users can examine the statistics in more detail, if they desire

# KOWWIN: Validation Data Set



# Running EPI Suite™



The screenshot shows the EPI Suite v3.20 application window. The title bar reads 'EPI v3.20'. The menu bar includes 'File', 'Edit', 'Functions', 'BatchMode', 'ShowStructure', 'Output', 'Capacity', 'STP', 'Other', and 'Help'. The main toolbar contains buttons for 'PhysProp', 'Previous', 'Get User', 'Save User', 'CAS Input', 'CALCULATE', 'ClearInputField', and 'What's New'. A large cyan arrow points to the 'CAS Input' button. Below the toolbar, there are several input fields: 'Enter SMILES:', 'Chem NAME', 'NameLooku', 'Henry LC (a', 'Water Dept', 'Wind Veloci', and 'Current Velocity(m/sec):'. A dialog box titled 'SMILECAS Database Retrieval' is open, featuring a text input field with '003380-34-5', 'OK' and 'Cancel' buttons, and an 'Output' section with 'Summary' (checked) and 'Full' (unchecked) options.



The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

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PhysProp

Previous

Get User

Save User

CAS Input

CALCULATE

ClearInputField

What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m3/mole):

River:

Water Depth (meters):

Wind Velocity (m/sec):

Current Velocity(m/sec):



The Estimation  
Protection Agency's Off  
(SRC). It is a screening  
tools, it is intended for  
release potential, and  
used when experimental (measured) values are available.

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### Chemical Name Lookup

Enter a chemical name ... the Name database will be searched for possible  
matches with corresponding SMILES notations.

Chemical Name:

OK

Cancel



PhysProp

Previous

Get User

Save User

CAS Input

CALCULATE

ClearInputField

What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m3/mole):

Water Depth (meters):

Wind Velocity (m/sec):

Current Velocity(m/sec):

## Names Found - Highlight and Select:

TRICLOSAN /003380-34-5  
3,4,5-TRICL-C6H2NHN=C(CN)CO-OME /036865-56-2  
2,4,5-TRICL-C6H2NHN=C(CN)CO-T-BU /028343-28-4  
A,A,B-TRICL-N-BUTYRALDEHYDE HYDRATE /000076-40-4  
TRICLOBISONIUM CHLORIDE /000079-90-3  
TRICLOCARBAN /000101-20-2  
TRICLOFOS /000306-52-5  
TRICLOPYR /055335-06-3  
TRICLOPYR BUTOXYETHYL ESTER /064470-88-8  
TRICLOPYR ESTER /064700-56-7  
TRICLOSAN /003380-34-5  
2(245-TRICL PH IMINO)IMIDAZOLIDINE /059465-40-6  
2(246-TRICL PH IMINO)IMIDAZOLIDINE /059465-51-9  
3,5,4'-TRICL SALICYLANILIDE /001151-51-5  
1-TRICONTANOL /000593-50-0  
12-TRICOSANAMINE, N,N-DIMETHYL- /071550-32-8  
TRICOSANE /000638-67-5  
METHYL N-TRICOSANOATE /002433-97-8

OK

Cancel

Prote  
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estim

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PhysProp Previous Get User Save User CAS Input CALCULATE ClearInputField What's New

Enter SMILES:   
003380-34-5

Chem NAME:   
NameLookup

Henry LC (atm-m3/mole):  Wat Sol (mg/L):

Vap Pr (mm Hg):

	River:	Lake:	Log Kow
Water Depth (meters):	<input type="text" value="1"/>	<input type="text" value="1"/>	
Wind Velocity (m/sec):	<input type="text" value="3"/>	<input type="text" value="0.5"/>	
Current Velocity(m/sec):	<input type="text" value="1"/>	<input type="text" value="0.05"/>	



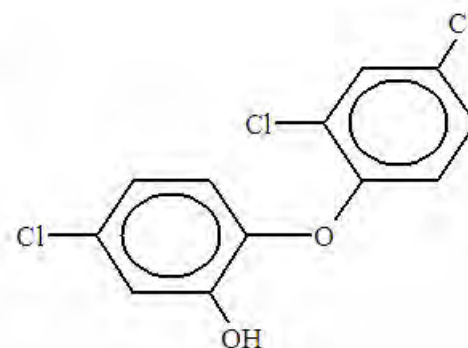
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### Structure

File Edit Structure Help



MolWt: 289.55 C<sub>12</sub> H<sub>7</sub> Cl<sub>3</sub> O<sub>2</sub>  
003380-34-5 Phenol, 5-chloro-2-(2,4-dic



EPI 3.20

File Functions BatchMode ShowStructure Output Fugacity STE

PhysProp Previous Get User Save User CAS Input CALCULATE

Enter SMILES: O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2  
003380-34-5

Chem NAME: Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-  
NameLookup

Henry LC (atm-m3/mole):

Water Depth (meters): 1  
Wind Velocity (m/sec): 3  
Current Velocity(m/sec): 1

River:



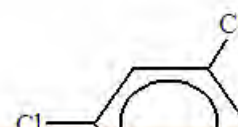
The Estimator Protection Agency's C (SRC). It is a screenin tools, it is intended for release potential, and used when experimen

Important infor estimation programs w

© 2000-2007 component programs

Structure

File Edit Structure Help



PhysProp Data

Print Copy TransferDataToEpiScreen

Experimental Data from PhysProp Database:

CAS Number: 003380-34-5  
Chem Name: 5-CHLORO-2-(2,4-DICHLOROPHENOXY)PHENOL  
MP (deg C): 54-57.3  
BP (deg C): ---  
Log Kow: 4.76  
Kow ref: CHEM INSPECT TEST INST (1992)  
Water Sol: 10 mg/L  
WS temp: 20 deg C  
WS ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)  
Vapor Pr: ---  
Henry LC: ---  
pKa: ---  
OH Rate: ---



PhysProp

Previous

Get User

Save User

CAS Input

CALCULATE

ClearInputField

What's New

Enter SMILES:  
003380-34-5O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2

Chem NAME:

Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-

NameLookup

Henry LC (atm-m3/mole):

Wat Sol (mg/L):

MP: 

Vap Pr (mm Hg):

BP: 

River:

Lake:

Log Kow: 

Water Depth (meters):

Wind Velocity (m/sec):

Current Velocity(m/sec):

Output

 Summary Full

The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

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## EPI Results

Print EPA\_upload Save Results Copy Help

SMILES : O(c(c(O)cc(c1)CL)c1)c(c(cc(c2)CL)CL)c2  
CHEM : Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-  
CAS NUM: 003380-34-5  
MOL FOR: C12 H7 CL3 O2  
MOL WT : 289.55

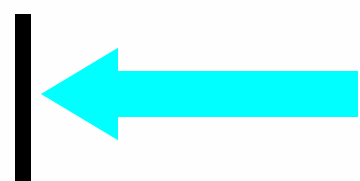
----- EPI SUMMARY (v3.20) -----

Physical Property Inputs:

Water Solubility (mg/L): 10  
Vapor Pressure (mm Hg) : -----  
Henry LC (atm-m<sup>3</sup>/mole) : -----  
Log Kow (octanol-water): 4.76  
Boiling Point (deg C) : -----  
Melting Point (deg C) : 54.00

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = 4.66  
Log Kow (Exper. database match) = 4.76  
Exper. Ref: Chem Inspect Test Inst (1992)



Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.42):

Boiling Pt (deg C): 373.62 (Adapted Stein & Brown method)  
Melting Pt (deg C): 136.79 (Mean or Weighted MP)  
UP(mm Hg,25 deg C): 4.65E-006 (Modified Grain method)  
MP (exp database): 54-57.3 deg C  
Subcooled liquid UP: 8.61E-006 mm Hg (25 deg C, Mod-Grain method)

# Full KOWWIN Output for Triclosan

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	12	Aromatic Carbon	0.2940	3.5280
Frag	3	-CL [chlorine, aromatic attach]	0.6445	1.9335
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-O- [aliphatic O, two aromatic attach]	0.2923	0.2923
Factor	1	Ortho-sub on di-aromatic ether (non-cyl)	-0.8396	-0.8396
Const		Equation Constant		0.2290

Log Kow = 4.6630

# EPI 2006 enhancements: octanol/air partition coefficient ( $K_{OA}$ ) via KOAWIN model

- $K_{OA} = \text{Conc. in } n\text{-Octanol} / \text{Conc. in Air}$   
Importance (uses in prediction):
  - Soil - Air partitioning
  - Vegetation - Air partitioning
  - Aerosol - Particulate partitioning
  - Bioaccumulation by terrestrial biota
  - Long-range transport potential (LRTP)

## EPI 2006 enhancements: fraction of airborne substance on particles ( $\phi$ ), via AEROWIN

- Distribution of an airborne chemical between particulate and gas phases is a key factor controlling photooxidation and deposition
- Fraction of chemical in the particulate phase ( $\phi$ ) is highly dependent upon VP
- Reactivity of particle-bound chemicals is poorly understood. It is generally assumed, but not always true, that bound chemical is unreactive

# Summary Output for AEROWIN and AOPWIN: Triclosan

## Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 0.00115 Pa (8.61E-006 mm Hg)

Log Koa (Koawin est ): 11.450

Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):

Mackay model : 0.00261

Octanol/air (Koa) model: 0.0692

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.0862

Mackay model : 0.173

Octanol/air (Koa) model: 0.847

## Atmospheric Oxidation (25 deg C) [AOPWIN v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 16.1147 E-12 cm<sup>3</sup>/molecule-sec

Half-Life = 0.664 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Half-Life = 7.965 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

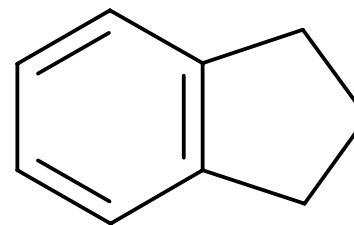
Reaction With Nitrate Radicals May Be Important!

**Fraction sorbed to airborne particulates (phi): 0.13 (Junge,Mackay)**

**Note: the sorbed fraction may be resistant to atmospheric oxidation**

# BioHCWIN v1.01

## Sample Results: Indane



TYPE	NUM	LOG Hydrocarbon FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic-CH2	0.1774	0.3548
Frag	4	Aromatic-H	0.0419	0.1678
Frag	1	-CH2- [cyclic]	0.0888	0.0888
Frag	1	Number of fused acyclic rings	0.5817	0.5817
Frag	1	Number of fused 6-carbon aromatic rings	0.0887	0.0887
Frag	1	Indane	-1.3080	-1.3080
Const	*	Equation Constant		0.4898
RESULT		LOG BioHC Half-Life (days)		0.4635
RESULT		BioHC Half-Life (days)		2.907

# Other EPI Suite™ Programs

## **ECOSAR**



- Discussed in Tala Henry's poster
- Library of QSARs for predicting aquatic toxicity and an Expert System for selecting the appropriate QSAR
- Runs automatically as integral part of EPI Suite™; also available by free download at:  
[www.epa.gov/oppt/newchems/tools/21ecosar.htm](http://www.epa.gov/oppt/newchems/tools/21ecosar.htm)


## **Dermwin v1.43**

- Dermal permeability coefficient from log Kow (KOWWIN)
- Runs only from EPI Suite™ subdirectory, not data entry screen





# EPI Suite™: Appropriate Use

 **EPI v3.20**

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp

Previous

Get User

Save User

CAS Input

CALCULATE

ClearInputField

What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m<sup>3</sup>/mole):

Wat Sol (mg/L):

MP:

Vap Pr (mm Hg):

BP:

Water Depth (meters):

River:

Lake:

Log Kow:

Wind Velocity (m/sec):

Current Velocity(m/sec):

0.5

0.05

Output

Summary

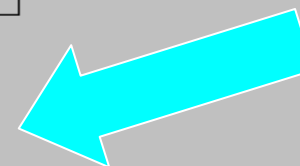
Full



The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

Important information on the performance, development and application of the individual estimation programs within EPI Suite™ is included in the User's Guide.

© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.



# EPI Suite™: Data Quality

The screenshot displays the EPI Suite v3.20 software interface. On the left is a vertical sidebar with input fields for 'Enter SMILES:', 'Chem NAME:', 'NameLookup', 'Henry LC (atm-m3/mole)', 'Water Depth (meters):', 'Wind Velocity (m/sec):', and 'Current Velocity(m/sec):'. Below these fields is the EPA logo and a partially visible text box containing 'Pro (SR tool rele use esti con'. The main window is titled 'Epi Suite Help' and contains a table of contents with 'Contents', 'Index', 'Back', and 'Print' buttons. The active section is '1.5. Data Quality Considerations', which contains two paragraphs of text. The first paragraph discusses the sources and quality control of data used in the software. The second paragraph details the periodic updates from the PHYSPROP database and the rigorous quality control process involving scientific evaluation and comparison of measured values to estimated values from various sources.

**EPI v3.20** | **Epi Suite Help**

File Edit Functions B: | File Edit Bookmark Options Help

PhysProp | Previous | Contents | Index | Back | Print

### 1.5. Data Quality Considerations

The User Guides for the individual estimation programs contain detailed information on the estimation methods, including sources of experimental data, predictive algorithms and method error (accuracy). The User Guides also reference publications in peer-reviewed journals in which further details are given. Most EPI Suite™ methods have been published in peer-reviewed journals. In general, measured values used to develop models were selected based on a multi-step review by senior scientists at Syracuse Research Corporation. In some cases, such as for the KOWWIN and WSKOW programs, most data came from highly regarded sources (e.g. Hansch et al. 1995) for which the data had already been carefully evaluated using explicit data quality criteria. For the KOWWIN program full reference citations are also given for all of the training set data. This allows users to check measured values themselves.

Measured values in the PHYSPROP file (accessed within EPI Suite™) are periodically uploaded from the PHYSPROP database maintained at Syracuse Research Corporation. This latter file has been actively built by SRC over the last two decades. It started as a database of physical properties for chemicals being evaluated by SRC for the Hazardous Substances Data Bank (HSDB), available from the National Library of Medicine (NLM)(<http://toxnet.nlm.nih.gov/>). Initially data were entered by junior and senior scientists using many sources for which the data had already been carefully evaluated (see Boethling RS, PH Howard and W Meylan. 2004. Finding and estimating chemical property data for environmental assessment. Environ. Toxicol. Chem. 23: 2290-3308). Data were then checked by senior scientists as described for the CHEMFATE file of the Environmental Fate Data Base (EFDB). For all records the QC process includes evaluation of the record to determine if the value makes sense scientifically (correct units, appropriate value given the chemical structure, etc). In addition, for approx. 10% of the records, a senior scientist checks the original source of the data. Additional quality control is performed by comparing measured values to estimated values from structure/property relationships (as a possible means of identifying outlying observations); and/or by comparing the values for one property (e.g. Henry's Law constant) to estimates derived from other properties (e.g., the ratio of vapor pressure and water solubility in the case of Henry's law constant - discussed in the preceding reference). This file is continually updated.

Pro (SR tool rele use esti con

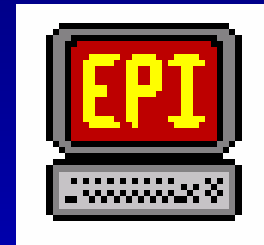
# 2005/6 Science Advisory Board (SAB) Review of EPI Suite™

- The charge: evaluate
  - The supporting science for comprehensiveness, accuracy, validation
  - Functionality: program documentation, user interface, etc
  - Whether EPI Suite™ is being used appropriately
- The SAB concluded that
  - EPI Suite™ is based on sound science and is user friendly, transparent, cost effective
  - Accuracy is sufficient to support regulatory screening
  - Numerous changes can be made to enhance scope, accuracy, ease of use
- December 2006 “Quality Review Draft” available at [www.epa.gov/sab/panels/epi\\_suite\\_review\\_panel.htm](http://www.epa.gov/sab/panels/epi_suite_review_panel.htm)

# EPI Suite™ Enhancements 2007/2008

- Existing programs: update
  - PCKOCWIN; HYDROWIN
- Add new properties and models
  - Bioaccumulation factor (BAF) and “Apparent  $K_m$ ” (fish metabolism) model to BCFWIN; add  $pK_a$
- Model accuracy issues
  - Domain; uncertainty; confidence interval; validation
- Transparency issues
  - Help files; international units; temperature dependence; complex mixtures
- Functionality—many SAB suggestions
  - Example: add ability to launch individual programs from main EPI screen

# For More Information



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- Philip Howard            howardp@syrres.com

- Internet

- Latest version (v3.20) dated Feb 2007
- *FREE* download at  
<http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>