

**RESOURCES FOR CONSULTANTS**

**A ROUND TABLE DISCUSSION**

**January 13, 2010**

**John Newport**



**chemventive**  
innovative excellence

## OVERVIEW

### OBJECTIVE :

To provide an update of Resources for  
Chemical Consultants

Information presented is supplemental to that  
already covered on the CCN website.

Emphasis on free/low cost resources.

### TOPICS

Finding work  
Searching for Information  
Databases  
Software  
News  
Business  
Educational

## FINDING WORK

**YOUR CCN WEB PAGE (Let the world find you) KEEP YOUR PAGE CURRENT AND COME TO CCN MEETINGS.**

**REGISTER AS A GOVERNMENT CONTRACTOR AT CCR.GOV.  
LOOK FOR OPPORTUNITIES AT FBO.GOV  
(FULL DETAILS IN OCT 14, 2009 CCN PRESENTATION)**

**IDEACONNECTION.COM**

REGISTER AS A SOLVER. ALSO, Online Data Services Ltd. will promote your consulting service on the IdeaConnection [website](#) to our 1 million plus yearly visitors.

All leads resulting from this online profile will be auto-forwarded instantly to you. Add IdeaConnection's innovation services to your toolkit and receive a great commission on each sale.

We agree to pay you 35% of all work you bring to us, and we would like you to pay us 7% of all

## SEARCHING FOR INFORMATION

[CHEMSPIDER.COM](http://CHEMSPIDER.COM)

[QUERTLE.COM](http://QUERTLE.COM)

[WOLFRAMALPHA.COM](http://WOLFRAMALPHA.COM)

[EMOLECULES.COM](http://EMOLECULES.COM)

[ORGANICWORLDWIDE.NET](http://ORGANICWORLDWIDE.NET)

[WWW.IBRIDGENETWORK.ORG](http://WWW.IBRIDGENETWORK.ORG)

## CHEMSPIDER

ChemSpider is a free access service providing a structure centric community for chemists. Providing access to millions of chemical structures and integration to a multitude of other online services, ChemSpider is the richest single source of structure -based chemistry information.

**Input a chemical name or structure and get detailed information on:**

Wikipedia Article(s)

Associated Data Sources and Commercial Suppliers

Patents (US, EP, WO, JP)

Experimental physchem properties

Names and Synonyms

ACD/Labs Predicted Properties (The standalone program costs \$12K)

Estimation Program Interface (suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention)

Spectral Data

## ACD/Labs Predicted Properties

<b><u>ACD/LogP</u></b>	3.82	<b># of Rule of 5 Violations:</b>	0
<b><u>ACD/LogD (pH 5.5):</u></b>	3.82	<b><u>ACD/LogD (pH 7.4):</u></b>	3.82
<b>ACD/BCF (pH 5.5):</b>	471.19	<b>ACD/BCF (pH 7.4):</b>	471.19
<b>ACD/KOC (pH 5.5):</b>	2851.54	<b>ACD/KOC (pH 7.4):</b>	2851.54
<b>#H bond acceptors:</b>	2	<b>#H bond donors:</b>	0
<b>#Freely Rotating Bonds:</b>	2	<b>PolarSurface Area:</b>	24.72 Å <sup>2</sup>
<b>Index of Refraction:</b>	1.574	<b>Molar Refractivity:</b>	58.85 cm <sup>3</sup>
<b>Molar Volume:</b>	178.1 cm <sup>3</sup>	<b>Polarizability:</b>	23.33 10 <sup>24</sup> cm <sup>3</sup>
<b>Surface Tension:</b>	39.8 dyne/cm	<b>Density:</b>	1.02 g/cm <sup>3</sup>
<b>Flash Point:</b>	122.9 °C	<b>Enthalpy of Vaporization:</b>	51.12 kJ/mb
<b>Boiling Point:</b>	293 °C at 760 mmHg	<b>Vapour Pressure:</b>	0.0031 mmHg at 25°C

# EPI Summary

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = 4.11

Log Kow (Exper. database match) = 3.82

Exper. Ref: Hansch,C et al. (1995)

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

Boiling Pt (deg C): 294.03 (Adapted Stein &  
Brown method)

Melting Pt (deg C): 13.57 (Mean or Weighted  
MP)

VP (mm Hg, 25 deg C): 0.0011 (Modified Grain  
method)

MP (exp database): 68.5 deg C

BP (exp database): 293 deg C

VP (exp database): 3.61E-04 mm Hg at 25 deg C

Subcooled liquid VP: 0.000972 mm Hg (25 deg C,  
exp database VP )

Water Solubility Estimate from Log Kow (WSKOW  
v1.41):

Water Solubility at 25 deg C (mg/L): 10.86

log Kow used: 3.82 (expkow database)

no-melting pt equation used

Water Sol (Exper. database match) = 6.4 mg/L  
(25 deg C)

Exper. Ref: TAKAGISHI,T ET AL (1969)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 6.3999 mg/L

Wat Sol (Exper. database match) = 6.40

Exper. Ref: TAKAGISHI,T ET AL (1969)

ECOSAR Class Program (ECOSAR v0.99h):

Class (es) found:

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:  
Bond Method : 1.47E -005 atm -m3/mole  
Group Method: 1.54E -005 atm -m3/mole  
Exper Database: 1.35E -05 atm -m3/mole  
Henrys LC [VP/WSol estimate using EPI values]:  
2.429E -005 atm -m3/mole

Log Octanol -Air Partition Coefficient (25 deg C)  
[KOAWIN v1.10]:  
Log Kow used: 3.82 (exp database)  
Log Kaw used: -3.258 (exp database)  
Log Koa (KOAWIN v1.10 estimate): 7.078  
Log Koa (experim ental database): None

Probability of Rapid Biodegradation (BIOWIN  
v4.10):  
Biowin1 (Linear Model) : 0.6751  
Biowin2 (Non -Linear Model) : 0.0148  
Expert Survey Biodegradation Results:  
Biowin3 (Ultimate Survey Model): 2.5401  
(wee ks -months)  
Biowin4 (Primary Survey Model) : 3.5418  
(days -weeks )  
MITI Biodegradation Probability:  
Biowin5 (MITI Linear Model) : 0.2063  
Biowin6 (MITI Non -Linear Model): 0.0000  
Anaerobic Biodegradation Probability:  
Biowin7 (Anaerobic Linear Model): 0.3181  
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):  
Structure incompatible with current estimation  
method!

Sorption to aerosols (25 Dec C) [AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 0.13 Pa  
(0.000972 mm Hg)  
Log Koa (Koawin est ): 7.078  
Kp (particle/gas partition coef. (m3/ug)):  
Mackay model : 2.31E -005

Octanol/air (Koa) model: 2.94E -006  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model : 0.000835  
Mackay model : 0.00185  
Octanol/air (Koa) model: 0.000235

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

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 1.5454 E -12  
cm<sup>3</sup>/molecule-sec  
Half-Life = 6.921 Days (12 -hr day; 1.5E6  
OH/cm<sup>3</sup>)

Half-Life = 83.056 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):  
0.00134 (Junge,Mackay)

Note: the sorbed fraction may be resistant to  
atmospheric oxidation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 1954  
Log Koc: 3.291

## Why Quertle is Different

**It's easy** - Quertle's friendly interface makes it simple to search and refine results .

**It's powerful** - Using its advanced LINGUISTICS, Quertle finds quality search results, not just long lists.

**It's inclusive** - All of PubMed (MEDLINE) **plus** an ever increasing number of full -text documents.

### Applied Filters

None

#### Published Within

Last 30 days

Last year

Last 3 years

Last 5 years

#### Publication Type

Reviews

Clinical Trials

Full-Text Documents

» More

### Key Concepts (for a search on Diffusion)

coefficient

wall

model

time

rate

H2O

image

concentration

protein

molecular

» More

(Contrast Scirus and Google Scholar)

<b>Organic Chemistry Literature</b>		
<a href="#">Bibliographic Databases</a>	<a href="#">Patents</a>	<a href="#">Text Books</a>
<a href="#">Reaction Databases</a>	<a href="#">Dissertations</a>	<a href="#">Reference Works</a>
<a href="#">Factual Databases</a>	<a href="#">Proceedings</a>	<a href="#">Current Awareness</a>
<a href="#">Articles</a>	<a href="#">Reviews</a>	<a href="#">Guides</a>
<a href="#">Journals</a>	<a href="#">Books</a>	<a href="#">Impact</a>
<b>Synthesis Planning</b>		
<a href="#">Retrosynthesis</a>	<a href="#">Reaction Prediction</a>	<a href="#">Library Design</a>
<b>Chemical Sourcing</b>		
<a href="#">Chemical Suppliers</a>	<a href="#">Compound Libraries</a>	<a href="#">Chemicals wanted/for sale</a>
<a href="#">Combined Catalogues</a>	<a href="#">Custom Synthesis</a>	<a href="#">Stockroom Inventory</a>
<b>Compound Classes</b>		
<a href="#">Peptides</a>	<a href="#">DNA and RNA</a>	<a href="#">Macrocycles</a>
<a href="#">Carbohydrates</a>	<a href="#">Isotopes</a>	<a href="#">Dendrimers</a>
<b>Synthesis Strategies</b>		
<a href="#">Asymmetric Synthesis</a>	<a href="#">Fluorous Chemistry</a>	<a href="#">Protecting Groups</a>
<small>Experimental Set -up and Purification</small>		
<b>Reaction Components</b>		
<a href="#">Heterogeneous Catalysts</a>	<a href="#">Organocatalysts</a>	<a href="#">Solvents</a>
<a href="#">Phase -Transfer Catalysts</a>	<a href="#">Biocatalysts</a>	<a href="#">Ionic Liquids</a>
<a href="#">Metal Catalysts/Ligands</a>	<a href="#">Reagents</a>	<a href="#">Supercritical Fluids</a>
<b>Reaction Activation</b>		
<a href="#">Microwave Synthesis</a>	<a href="#">Sonochemistry</a>	<a href="#">Electrosynthesis</a>
<a href="#">Photochemistry</a>	<a href="#">Mechanochemistry</a>	
<b>Reaction Set -up</b>		
<a href="#">Reaction Blocks/Workstations</a>	<a href="#">Glassware</a>	<a href="#">Continuous Flow</a>
<a href="#">Robotarm -based Systems</a>	<a href="#">Thermometers</a>	<a href="#">Dispensers</a>
<a href="#">Stirrers</a>	<a href="#">Balances</a>	<a href="#">Laboratory Techniques</a>
<b>Safety</b>		
<a href="#">MSDS</a>	<a href="#">Toxicity</a>	<a href="#">Waste Disposal</a>

## Work-up and Purification

<a href="#">Evaporation</a>	<a href="#">Liquid-Liquid Extraction</a>	<a href="#">Membrane Filtration</a>
<a href="#">Solid Phase Extraction</a>	<a href="#">Preparative Chromatography</a>	<a href="#">Pervaporation</a>

### Structure Confirmation

## Structural Analysis and Detection

<a href="#">NMR</a>	<a href="#">Gas Chromatography</a>	<a href="#">Mass Spectrometry</a>
<a href="#">Infrared Spectroscopy</a>	<a href="#">HPLC</a>	<a href="#">Vibrational Circular</a>
<a href="#">UV/Visible</a>	<a href="#">Ion Chromatography</a>	<a href="#">Dichroism</a>
		<a href="#">ELSD</a>

## Physico-Chemical Properties

<a href="#">Melting Point</a>	<a href="#">pKa and pKb</a>	<a href="#">LogP</a>
<a href="#">Boiling Point</a>	<a href="#">Solubility</a>	<a href="#">Optical Rotation</a>

### Reporting and Communication

## The Desk

<a href="#">Notebooks</a>	<a href="#">Drawing/Visualization</a>	<a href="#">Nomenclature</a>
<a href="#">Writing</a>	<a href="#">Classification</a>	<a href="#">Tutorials</a>

## Communication

<a href="#">Conferences</a>	<a href="#">Courses</a>	<a href="#">Research groups</a>
<a href="#">Exhibitions</a>	<a href="#">Cybercommunication</a>	<a href="#">Chemical Organizations</a>

## Additional Activities for Organic Chemists

<a href="#">Jobs</a>	<a href="#">Ideas</a>	<a href="#">Brain Relaxation</a>
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# IBRIDGENETWORK.ORG

The iBridge<sup>SM</sup> Network provides a public, centralized source for unbiased information about early stage technologies and inventions.

Through the iBridge<sup>SM</sup> Network, researchers and those seeking innovations can easily search for and obtain the resources they need.

# WOLFRAMALPHA

*Making the World's Knowledge Computable*

Today's Wolfram|Alpha is the first step in an ambitious, long-term project to make all systematic knowledge immediately computable by anyone. Enter your question or calculation and Wolfram|Alpha uses its built-in algorithms and a growing collection of data to compute the answer. Based on a new kind of knowledge-based computing...

Sample Input: **Chemists salaries**

Input interpretation:

US chemists

median wage

annual

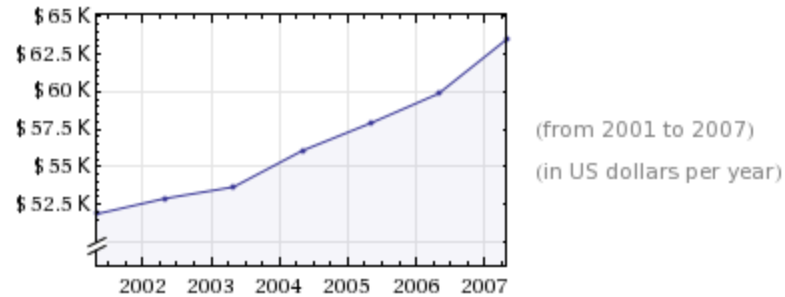
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Result:

\$63 490 per year (2007 estimate)

## History:



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## US employment summary: [More](#)

people employed	79 860 people (1 in 1682)
yearly change	- 640 people (-0.8%)
median wage	\$63 490 per year
yearly change	+\$3620 per year (+6.0%)
50% range	\$47 050 to \$85 960 per year
80% range	\$36 810 to \$108 600 per year

(2007 data)

Sample Input:  $y''(x)+x*y=0$

Input: [Mathematica form](#)

$$y''(x) + x y(x) = 0$$

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ODE classification:

Second-order linear ordinary differential equation

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Differential equation solution:

$$y(x) = c_1 \operatorname{Ai}\left(\sqrt[3]{-1} x\right) + c_2 \operatorname{Bi}\left(\sqrt[3]{-1} x\right)$$

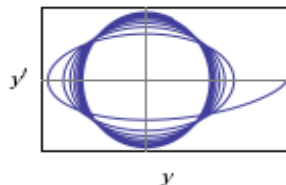
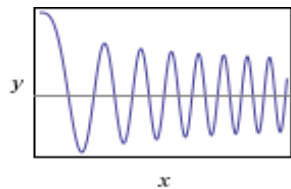
$\operatorname{Ai}(x)$  is the Airy function» | [Documentation](#) | [Properties](#) | [Definition](#)

$\operatorname{Bi}(x)$  is the Airy Bi function» | [Documentation](#) | [Properties](#) | [Definition](#)

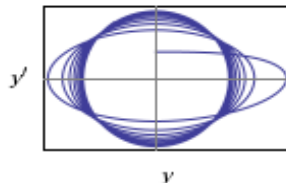
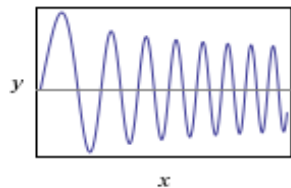
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Plots of sample individual solutions:



$$y(0) = 1$$
$$y'(0) = 0$$



$$y(0) = 0$$
$$y'(0) = 1$$

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## Sample Input: Ethanol 12 5C

Input interpretation:

- [Mathematica form](#)

ethanol	temperature	125 °C (degrees Celsius)
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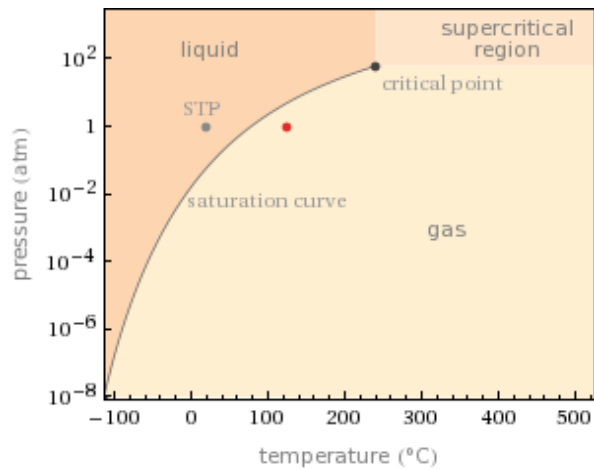
Thermodynamic properties:

- [More](#)

phase	gas
density	1.435 kg/m <sup>3</sup> 0.001435 g/cm <sup>3</sup>
boiling point	78.29 °C
molar volume	32 108 cm <sup>3</sup> /mol
sound speed	622.7 mph 278.4 m/s
specific acoustic impedance	399.4 s Pa/m

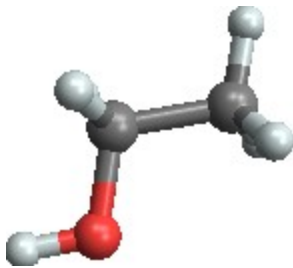
(assuming 1 atm)

## Phase diagram:



## 3D structure:

- [Show space filling](#)



## Basic properties:

## DATABASES

### CHEMICAL REGISTER.COM

Database of Chemical Industry Suppliers

### DNB.COM DUNN & BRADSTREET

Business and business credit database

SCOPUS.COM abstract and citation  
database of research literature.

### POLYSACCHARIDECENTER.COM

Chemical and physical properties of  
polysaccharides

### ELECTROCHEMISTRY ENCYCLOPEDIA

<http://electrochem.cwru.edu/encycl/>

Covers many aspects of electrochemistry,  
electroanalytical chemistry, electrochemical  
engineering, and electrochemical  
technology .

<http://www.chemtube3d.com/>

This site contains interactive 3D animations  
for some of the most important organic  
reactions with supporting information on  
reactivity and spectroscopy.

## SOFTWARE

### [OPENBABEL.COM](http://openbabel.com)

Open Babel is An Open Source chemical toolbox designed to speak the many languages of chemical data. It's a collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.

### [MEGAUPLOAD.COM](http://megaupload.com)

For sending and receiving very large files

### **[ACD/ChemSketch 12.0 Freeware](http://acdlabs.com/download/chemsketch/)**

<http://acdlabs.com/download/chemsketch/>

**A Comprehensive Chemical Drawing Package**

### [CHEMISTRY-BLOG.CPM/DICTIONARY/](http://chemistry-blog.cpm/dictionary/)

**Chemistry Dictionary for Word Processors – Version 2.0 (Updated)**

## NEWS

### [U2M Financial News Aggregator](#)

**Aggregates news from CNBC, Google, Yahoo, CNN, Business Week, Smart Money and Bloomberg TV.**

### [BOILTHISDOWN.ORG](#)

**ACS site that reviews chemical and industry news on a daily basis.**

### [NATURE PRECEEDINGS](#)

<http://precedings.nature.com/>

**Nature Precedings provides a platform for sharing new and preliminary findings with colleagues on a global scale.**

**Post pre-print manuscripts, posters and presentations on Nature Precedings to claim priority and receive feedback on your findings prior to formal publication.**

## BUSINESS

Outright is a free software -as-a-service described as a "dead simple online bookkeeping designed specifically for self-employed folks."

Tracks income and expenses and groups them in categories that the IRS wants to see and fills out a Schedule C.

### **GOOGLE VOICE (BY INVITATION)**

No internet connection needed for calls

Use Google Voice with your existing number <sup>new!</sup> and get:

- Google voicemail: voicemail like email
- Voicemail transcription: read what your voicemail says
- Custom greetings: vary voicemail greetings by caller
- International calling: low cost calls to the world Notifications: read voicemail messages via email or SMS
- Share voicemails: forward, embed, or download voicemails

**Add a Google number to get these **additional** features:**

- **One number:** a single phone number that rings all your phones
- **Free SMS:** send, receive & store text messages online (free domestic)
- **Block calls:** send unwanted callers straight to voicemail
- **Record calls:** record phone calls and store them online
- **Conference calls:** join several people into a single call
- **Screen callers:** hear who is calling before you pick up

### **[SKYPE.COM](http://SKYPE.COM)**

**Low cost national and international plans to landlines and mobile phones (need internet connection)**

**Euros/month 1.95 (Domestic) 3.95 (Country) 8.95 (World) (Free: Skype to Skype)**

### **[VYEW.COM](http://VYEW.COM)**

**Anyone can host a web session where colleagues can work together on a project in real time. Provides a very simple whiteboard where you can upload documents for discussion. (Free for up to 20 users)**

### **[GOOGLE WAVE](http://GOOGLE WAVE)**

**Communicate and collaborate in real time (currently in limited preview – by invitation)**

### **[LABX.COM](http://LABX.COM)**

**For used Scientific equipment by sale or auction.**

### **[CONSULTINGPULSE.COM](http://CONSULTINGPULSE.COM)**

**Consulting newsletter**