## Range of Henry's Law Constants



## Air partitioning increases

## Water partitioning increases

Figure 6.2 Ranges in Henry's Law constants $\left(K_{H}\right)$ for some important classes of organic compounds.

## Relative range in values

## solubility

## Vapor pressure

## Henry's coefficient



Ranges in water solubilities $\left(C_{\mathrm{w}}^{5 \text { st }}\right)$ of some important classes


Ranges at $25^{\circ} \mathrm{C}$ in saturation vapor pressure ( $\rho^{\circ}$ ) values for some janic compounds.


Ranges in Henry's Law constants ( $K_{H}$ ) for some important classes of C

## Presentations: powerpoint on go/echem

- 15 minutes +5 for questions
- Paper of your choosing, approved by me
- Environmental Science \& Technology (ACS)
- Organic compounds in the environment
- Chemistry \& Experimental focus
- Sources beyond the article are expected
- Textbooks/online sources to refine understanding of terms, particularly in the Methods section, as needed
- at least 2 important sources cited in the Discussion of your article - integrate other literature findings that your article is being interpreted in light of


## Intermolecular force LFER for $\mathbf{K}_{\mathrm{H}}$

$$
\ln \gamma_{i w}=-\ln p_{i L}^{\circ}-0.572\left[\left(V_{i}\right)^{2 / 3}\left(\frac{n_{D i}^{2}-1}{n_{D i}^{2}+2}\right)\right]-5.78 \pi_{i}-8.77\left(\alpha_{i}\right)-11.1\left(\beta_{i}\right)+0.0472 V_{i}+9.49
$$

$$
\ln K_{i, h}(-)=-0.540\left[\left(V_{i}\right)^{2 / 3}\left(\frac{n_{D i}^{2}-1}{n_{D i}^{2}+2}\right)\right]-5.71 \pi_{i}-8.74 \alpha_{i}-11.2 \beta_{i}+0.0459 V_{i}+2.25
$$

London dispersion forces $\mathrm{n}_{\mathrm{D}}=$ refractive index (polarizability, Table 3.1)

Dipolar (HDA) interactions $\pi=$ "pi term" (Table 5.5)

HDA interactions
H-donor ( $\alpha$ ) \& H acceptor ( $\beta$ ) terms (Table 4.3)

Entropy/size
Volume term

## $\mathrm{K}_{\mathrm{H}}$ resources

Environ. Sci. Technol. 2010, 44, 352

# Genotoxicity of Water Concentrates from Recreational Pools after Various Disinfection Methods 

DANAE LIVIAC, ${ }^{+}$<br>ELIZABETH D. WAGNER, ${ }^{\ddagger}$<br>WILLIAM A. MITCH, ${ }^{\text {® }}$<br>MATTHEW J. ALTONJI, ${ }^{\S}$ AND<br>MICHAEL J. PLEWA* ${ }^{*}$

- Killer Showers
- Killer Hot Tubs
- EPA Estimator

http:/ /www.undercovercaterer.com/wp-content/uploads/2010/09/hot-tub.jpg


## Lindane Global Transport



- $\gamma$-HCH - a "toxic 21" POP
- $\mathrm{K}_{\mathrm{aw}}\left(25^{\circ} \mathrm{C}\right)=0.24 \mathrm{~Pa} \mathrm{~m} / \mathrm{mol}$
- $\Delta \mathrm{H}_{\mathrm{aw}}\left(25^{\circ} \mathrm{C}\right)=61400 \mathrm{~J} / \mathrm{mol}$
- $\mathrm{R}=8.314 \mathrm{~Pa} \mathrm{~m}^{3} /(\mathrm{mol} \mathrm{K})$

1,2,3,4,5,6-hexachlorocyclohexane
Compare $[\mathrm{L}]_{\mathrm{w}}$ in Lake Champlain $\left(25^{\circ} \mathrm{C}\right)$ near a farm that uses it on its crops with...
$[\mathrm{L}]_{w}$ in the $\operatorname{Arctic}\left(1^{\circ} \mathrm{C}\right)$
given that the $[\mathrm{L}]_{\mathrm{a}}$ is 100 and $10 \mathrm{pg} / \mathrm{m}^{3}$ in each location, respectively.

## Grasshopper effect: spatial \& temporal



Warmer areas
Net evaporation
higher $\mathrm{K}_{\mathrm{H}}$
(source)

Elevational, latitudinal
Daily, seasonal
Coastal/continental
http://www.ainc-inac.gc.ca/ai/scr/nt/images/nt/pop-pop-1-eng.jpg

## Global Distillation



- More volatile compounds are transported faster (atmosphere moves faster than ocean)

Journal of Exposure Science and Environmental Epidemiology (2006) 16, 207-224. doi:10.1038/sj.jes. 7500456

