Bisphenol A and public policy

"Although scientific inquiry is a dynamic give-and-take among researchers with different opinions and viewpoints, the socalled controversies surrounding low-dose effects and NMDR curves should be put to rest...These phenomena have been demonstrated time and again for a sufficient number of endocrine-related endpoints, and they no longer merit being considered "controversial" topics."

Vandenberg et al. Endocrine Reviews **2009**, *30*, 75. (authors from Tufts University School of Medicine)

Vapor Pressure Ranges



Schwarzenbach et al. Environmental Organic Chemistry, 1st ed., 1996

vp versus C-number



Schwarzenbach et al. Environmental Organic Chemistry, 1st ed., 1996

Intermolecular Forces and VPs



Schwarzenbach et al. Environmental Organic Chemistry, 2nd ed., 2003

Experimental log P^o vs. 1/T



Schwarzenbach et al. Environmental Organic Chemistry, 2nd ed., 2003

Clausius-Clapeyron Example

Consider 1,2,4,5-tetramethylbenzene (TeMB). In an old CRC, you find the following data



T_m = 79.5 °C T_b = 195.9 °C MW=134.2 g/mol

 Estimate vp (Pa) of TeMB at 20 °C and at 150 °C.
Also, express your answer in g/m³.

Beware of P & T units!!

Empirical Prediction of Heats of Vaporization and Heats of Adsorption of Organic Compounds

Kai-Uwe Goss, and Ren P. Schwarzenbach

Environ. Sci. Technol., 1999, 33 (19), 3390-3393• DOI: 10.1021/es980812j • Publication Date (Web): 24 August 1999

Downloaded from http://pubs.acs.org on March 12, 2009



Vapor Pressure Estimations



- 1. What is the vapor pressure of benzene at 30 °C? Given, $P_{L}^{o}(25^{\circ}C) = 10^{-0.9}$ atm?
- 2. What is the vapor pressure of benzyl alcohol at 25 °C, given $T_b = 205.3$ °C; $T_m = 15$ °C; 108.14 g/mol
- 3. What is the vapor pressure of benzene at 3 °C? $T_b = 80.1$ °C; $T_m = 5.5$ °C; 78.1 g/mol

1 atm = 101325 Pa R = 8.314 J/(mol K)

Toxic Contamination From Natural Gas Wells

"While the existence of the toxic wastes has been reported, thousands of internal documents obtained by The New York Times from the <u>Environmental Protection Agency</u>, state regulators and drillers show that the <u>dangers</u> to the environment and health are greater than previously understood."

Kevin Moloney, New York Times February 26, 2011

Governor of Maine on EDCs

"The only thing that I've heard is if you take a plastic bottle and put it in the microwave and you heat it up, it gives off a chemical similar to estrogen. So the worst case is some women may have little beards."

http://new.bangordailynews.com/2011/02/22/health/govlepage-dismisses-dangers-of-bpa/

> Paul LePage, Governor of ME February 2011

Moby Duck: 28,800 Toys at Sea

"But both the birth and the afterlife of the duck, Hohn soon learns, are toxic. Adrift on the ocean, the toys can become coated with "persistent organic pollutants" like polyvinyl chloride, bisphenol A and phthalates. Photodegraded into smaller pieces, they can be fatally ingested by sea creatures and will endure, in swirling gyres, for years. ."

> Ny Times Book Review "Moby Duck" February 2011

Empirical VP Estimations

- 1. Calculate τ & HBN for
 - Benzene
 - benzyl alcohol
 - Dichlorodiphenyl trichloroethane (DDT)
 - 2,4,7,8-tetrachlorodibenzodioxin
 - 2,4,7,8-tetrachloro diphenyl ether

Empirical VP Estimation: benzyl alcohol What is the vapor pressure of benzyl alcohol at 25 °C? 1. $T_{\rm b} = 205.3 \text{ °C}; T_{\rm m} = 15 \text{ °C}; 108.14 \text{ g/mol}$ units!! HBN $\ln P_{iL}^{\circ} = -\left[21.2 + 0.3(1.5) + 177(0.00925)\right] \left[\frac{205.3 + 273K}{298K} - 1 \right] +$ $+\left[\left[10.8 + 0.25(1.5) \right] \ln \left(\begin{array}{c} 205.3 + 273K \\ \hline 298K \end{array} \right) \right] = -8.80$ $P_{iL}^{\circ} = e^{-8.80} = 0.000150 bar$ units!! $P_{iL}^{\circ} = 0.000150 bar \frac{100000 Pa}{1 bar} = 15.0 Pa$

1 bar= 100,000 Pa

Empirical VP Estimation: benzene What is the vapor pressure of benzene at 3 °C? 1. $T_{\rm b} = 80.1 \text{ °C}; T_{\rm m} = 5.5 \text{ °C}; 78.1 \text{ g/mol}$ $\ln P_{iL}^{\circ}(bar) = -\left[(21.2 + 0.3)(1 + 177)(0)\right] \left(\frac{80.1 + 273K}{276K} - 1\right) +$ $\left| + \left[10.8 + 0.25 \right] \ln \left(\frac{80.1 + 273K}{276K} \right) \right] = -3.26$

$$P_{iL}^{\circ}(bar) = e^{-3.26} = 0.0383bar$$



Is this <u>really</u> the P⁰ for benzene at 3 °C?

Theoretical states...strange but useful

