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HPLC-Based Method for Estimating the Temperature Dependence of *n*-Octanol−Water Partition Coefficients

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Retention time measurements on reversed phase HPLC-columns over a 50 K temperature range are used to estimate the enthalpy of octanol−water phase transfer $\Delta_{OW}H$ for 38 organic compounds of environmental relevance, including selected chlorinated benzenes (CBzs), polycyclic aromatic hydrocarbons (PAHs), polychlorinated naphthalenes (PCNs) and biphenyls (PCBs). Literature K_{OW} values as a function of temperature for CBzs served as a reference. $\Delta_{OW}H$ for these compounds range from 13 to 32 kJ/mol, confirming a relatively minor temperature dependence of their partitioning between water and octanol. For the chlorinated aromatics a strong linear relationship between Δ_{OW}H and molar volume was observed. The temperature-dependent retention volumes are also used to estimate K_{OW} of selected PCNs and PAHs at 25 °C.

Introduction

The octanol−water partition coefficient K_{OW} is one of the most important partition coefficients in a pharmaceutical and environmental context. Traditional methods for determining K_{OW} are the shake flask (De Bruijn et al., 1989) and generator column technique (Woodburn et al., 1984). These techniques are very time and labor intensive. More rapid estimation of K_{OW} has been achieved by regressing a compound's K_{OW} with its retention on Reversed Phase − High Performance Liquid Chromatographic (RP-HPLC) columns (Veith et al., 1979; Könemann et al., 1979; McDuffie, 1981). The method has been improved upon and applied extensively (e.g. Hammers et al., 1982; Rapaport and Eisenreich, 1984; Kaune et al., 1995, Ritter et al., 1995). Although purely empirical, these HPLC-based methods have proven useful and sufficiently reliable for many applications. It is well established that partition coefficients are temperature dependent. Compared to the temperature dependence of partition coefficients between the vapor phase and a condensed phase, the temperature dependence of K_{OW} is relatively minor (Sangster, 1989) and therefore has not been quantified very often (James et al., 1981; Beezer et al., 1980, Paschke and Schüürmann, 1998). Notable exceptions are the studies by Opperhuizen et al. (1988) and more recently by Bahadur et al. (1997) reporting the temperature dependence of the K_{OW} of selected chlorobenzenes.

Here we present a novel method of rapidly estimating the enthalpy of octanol−water phase transfer $\Delta_{OW}H$, that is, the temperature dependence of K_{OW}, for organic compounds from retention time measurements on reversed phase HPLC-columns at variable temperature. The method requires a set of reference compounds with well-established K_{OW} and $\Delta_{OW}H$. When calibrated properly, temperature-dependent retention time values can also be used to estimate K_{OW} at 25 °C. The theoretical basis for the method, which is essentially an adaptation of the gas chromatographic retention time method for determining temperature-dependent vapor pressures of the supercooled liquid (Hamilton, 1978; Bidleman, 1984; Hinckley et al., 1990), is presented. The method is further employed to determine the Δ_{OW}H for 38 organic chemicals, specifically selected CBzs, PCBs, PCNs, and PAHs. K_{OW} at 25 °C for PCNs and four PAHs are estimated based on a calibration using the data for CBzs, PCBs and some PAHs.

Theory

The capacity factor k' for a substance on a chromatographic column is defined as

$$k' = (t_R - t_0)/t_0$$

where t_R is the compound's elution volume and t_0 is the void volume, or the elution volume of the mobile phase. t_0 is obtained by measuring the elution volume of a chemical that is not retained by the stationary phase. Estimation methods for the octanol−water partition coefficient K_{OW}, which are based on capacity factors in reversed phase HPLC columns, make use of the similarity between the partitioning process between *n*-octanol and water and that between the mobile and stationary phase used for determining the capacity factors. Between the K_{OW} values of a series of compounds and their capacity factor k', empirical relationships of the following type have been observed:

$$K_{OW} = Ak'^{B}$$

In logarithmic form

$$\ln K_{OW} = B \ln k' + \text{constant} \qquad (1)$$

that is a plot of ln K_{OW} against ln k' should give a straight line with slope B. Therefore, for a substance i with K_{OWi} and a reference substance with K_{OWref} eluted on the same HPLC column

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$$\ln K_{\mathrm{OW}i} = \ln K_{\mathrm{OWref}} + B \ln\left(\frac{k'_i}{k'_{\mathrm{ref}}}\right) \tag{2}$$

Further, the temperature dependence of K_{OW} can be expressed as

$$\frac{\mathrm{d} \ln K_{\mathrm{OW}}}{\mathrm{d}T} = \frac{\Delta_{\mathrm{OW}}H}{RT^2} \tag{3}$$

where $\Delta_{\mathrm{OW}}H$ is the enthalpy of phase transfer between octanol and water and T is temperature. Rewriting eq 3 for a substance i and a reference substance at the same temperature

$$\frac{1}{\Delta_{\mathrm{OW}}H_i}\,\mathrm{d} \ln K_{\mathrm{OW}i} = \frac{1}{RT^2}\,\mathrm{d}T$$

$$\frac{1}{\Delta_{\mathrm{OW}}H_{\mathrm{ref}}}\,\mathrm{d} \ln K_{\mathrm{OWref}} = \frac{1}{RT^2}\,\mathrm{d}T$$

that is

$$\mathrm{d} \ln K_{\mathrm{OW}i} = \frac{\Delta_{\mathrm{OW}}H_i}{\Delta_{\mathrm{OW}}H_{\mathrm{ref}}}\,\mathrm{d} \ln K_{\mathrm{OWref}}$$

Integration yields

$$\ln K_{\mathrm{OW}i} = \frac{\Delta_{\mathrm{OW}}H_i}{\Delta_{\mathrm{OW}}H_{\mathrm{ref}}} \ln K_{\mathrm{OWref}} + C \tag{4}$$

where C is the constant of integration. Combining eqs 2 and 4 gives

$$\ln K_{\mathrm{OWref}} + B \ln\left(\frac{k'_i}{k'_{\mathrm{ref}}}\right) = \frac{\Delta_{\mathrm{OW}}H_i}{\Delta_{\mathrm{OW}}H_{\mathrm{ref}}}\,\mathrm{d} \ln K_{\mathrm{OWref}} + C$$

and after rearranging

$$\ln\left(\frac{k'_i}{k'_{\mathrm{ref}}}\right) = \left(\frac{\Delta_{\mathrm{OW}}H_i}{\Delta_{\mathrm{OW}}H_{\mathrm{ref}}} - 1\right)\frac{\ln K_{\mathrm{OWref}}}{B} + \frac{C}{B} \tag{5}$$

A plot of $\ln(k'_i/k'_{\mathrm{ref}})$ versus $\ln K_{\mathrm{OWref}}/B$ should give a straight line with intercept C/B and slope $((\Delta_{\mathrm{OW}}H_i/\Delta_{\mathrm{OW}}H_{\mathrm{ref}}) - 1)$, where k'_i/k'_{ref} is the relative capacity factor at the temperature where the reference compound has the octanol−water partition coefficient K_{OWref}. Note that B is also a function of temperature and needs to be determined from regressions of measured $\ln k'$ values against known temperature-dependent K_{OW} values.

$\Delta_{\mathrm{OW}}H_i$ is then obtained from the regressed slope of eq 5 and $\Delta_{\mathrm{OW}}H_{\mathrm{ref}}$ using

$$\Delta_{\mathrm{OW}}H_i = (\mathrm{slope} + 1)\Delta_{\mathrm{OW}}H_{\mathrm{ref}} \tag{6}$$

It may be noteworthy that this method does not require the assumption that the temperature dependence of K_{OW} is identical to that of the capacity factor k'. In deriving eq 5 we only make use of eqs 2 and 4. Whereas eq 4 is valid independent of the retention time method, eq 2 assumes that the K_{OW} of a compound at one temperature can be obtained from that of a reference compound and the ratio of the capacity factors of the compound and the reference compound, as long as all parameters, that is, K_{OWref}, $K_{\mathrm{OW}i}$, B, k'_i, and k'_{ref}, refer to the same temperature.

Table 1. Parameters Used in the Interpretation of Temperature Dependent Elution Volumes on a RP-HPLC Column

	5 °C	15 °C	25 °C	35 °C	45 °C	55 °C
$\log K_{\mathrm{OWref}}$[a]	4.54	4.42	4.31	4.21	4.11	4.02
B[b]	2.449	2.492	2.514	2.615	2.671	2.765
$\ln K_{\mathrm{OWref}}/B$[c]	4.270	4.086	3.948	3.704	3.544	3.347

[a] These are values for the K_{OW} of 1,3,5-trichlorobenzene calculated from the regression reported from Bahadur et al. (1998), and not the measured values. [b] B was calculated by regressing measured temperature-dependent capacity factors k' against $\ln K_{\mathrm{OW}}$ values reported by Bahadur et al. (1998) [c] These values were employed in the regression equations (5).

Table 2. Enthalpy of Octanol−Water Phase Transfer $\Delta_{\mathrm{OW}}H$ for Selected Organic Compounds Estimated from Temperature Dependent Capacity Factors on a RP-HPLC Column

	$\Delta_{\mathrm{OW}}H$/kJ·mol^{-1}
chlorobenzenes	
benzene	13.3
monoCBz	15.0
1,2-diCBz	16.6
1,3-diCBz	16.9
1,4-diCBz	16.2
1,2,4-triCBz	18.1
1,2,3,4-tetraCBz	20.8
1,2,3,5-tetraCBz	19.9
1,2,4,5-tetraCBz	19.3
pentaCBz	22.0
hexaCBz	24.3
polychlorinated biphenyls	
4,4′-diCB	20.9
2,4,6-triCB	20.4
2,3,4,5-tetraCB	24.0
polycyclic aromatic hydrocarbons	
naphthalene	15.7
fluorene	19.0
anthracene	19.7
phenanthrene	19.0
fluoranthene	20.8
pyrene	19.2
chrysene	22.7
benzo[*a*]pyrene	25.4
benzo[*g*,*h*,*i*]perylene	27.7

It is also possible to estimate $K_{\mathrm{OW}i}$ from this regression. Combing eqs 2 and 5 yields

$$\ln K_{\mathrm{OW}i} = \left(\frac{\Delta H_{\mathrm{OW}i}}{\Delta H_{\mathrm{ref}}}\right) \ln K_{\mathrm{OWref}} + C \tag{7}$$

where $(\Delta_{\mathrm{OW}}H_i/\Delta_{\mathrm{OW}}H_{\mathrm{ref}}) = \mathrm{slope} + 1$ and $C = B(\mathrm{intercept})$.

Methods

Chemicals. Selected PAHs and CBzs (>99% purity or highest commercial quality) were obtained from Aldrich Chemical Co. (Milwaukee, WI), hexachlorobenzene (OAS grade) from BDH Chemicals Ltd. (Toronto, ON), and selected PCN congeners of unspecified, but high purity from Aldrich Chemical Co. (Milwaukee, WI), Wellington Laboratories (Guelph, ON) and Ultra Scientific (Kingstown, RI).

Instrumentation. A Waters Associates (Millford, MA) HPLC system consisting of a model U6K injector, model 6000 and M45 solvent delivery systems, a model 721 flow controller, and a model 440 UV absorbance detector with 254 nm kits was employed. Integration of peak area was recorded by a Waters 730 Data Module. The analytical column (Waters μBondapak-C18 column, 10 μm, 3.9 mm o.d. × 300 mm long) was placed in a water jacket and its temperature controlled by a refrigerated circulating bath (Endocal, RTE-5). For each chemical the capacity factor k' was determined at five to six temperatures in the range 5 °C to 55 °C. These experiments were run with isocratic

Table 3. Uncalibrated log $K_{OWexptl}$ and Calibrated log K_{OW} Values at 25 °C, log K_{OWlit} from the Literature, Parameter A for Eq 9, and the Enthalpies of Phase Transfer Octanol−Water $\Delta_{OW}H$ in for Selected PCNs and PAHs

	log $K_{OWexptl}$	log K_{OW}	log $K_{OW\ lit}$	A	$\Delta_{OW}H$/kJ·mol^{-1}
2-methylanthracene	4.70 ± 0.01	4.97		1.093	22.1
triphenylene	4.83 ± 0.01	5.15	5.49,[a] 5.84[b]	1.313	21.8
benz[*a*]anthracene	4.98 ± 0.01	5.33	5.79,[a] 5.84,[b] 5.91[c]	1.238	23.3
benz[*e*]acephenanthrylene	5.36 ± 0.01	5.82	5.78[a]	1.371	25.4
1-monoCN	3.97 ± 0.00	4.0	3.90[e]	0.841	18.0
2-monoCN	3.91 ± 0.00	3.9	4.19,[d] 3.98[e]	0.821	17.7
1,2-diCN	4.45 ± 0.00	4.6	4.40,[d] 4.42[e]	1.064	20.3
1,4-diCN	4.57 ± 0.00	4.8	4.88,[d] 4.66[e]	1.269	20.1
1,2,3,4-tetraCN	5.76 ± 0.00	6.3	5.94,[d] 5.75[e]	1.832	25.8
1,2,3,5,8-pentaCN	6.13 ± 0.00	6.8		2.035	27.4
1,2,3,4,6-pentaCN	6.27 ± 0.01	7.0		2.166	27.7
1,2,3,5,7,8-hexaCN	6.69 ± 0.00	7.5		2.413	29.4
1,2,3,4,6,7-hexaCN	6.79 ± 0.01	7.7		2.489	29.8
1,2,3,4,5,6,7-heptaCN	7.18 ± 0.01	8.2		2.638	31.8
octaCN	7.46 ± 0.01	8.5	8.40,[d] 6.42[e]	2.998	31.8

[a] Wang et al., 1986. [b] De Voogt et al., 1990. [c] Miller et al., 1985. [d] Opperhuizen et al., 1985. [e] Opperhuizen, 1987.

elution. The eluent (flow rate 1.1 mL/min) was 81% methanol (HPLC grade, Caledon Laboratory Chemicals, Georgetown, Ont.) in water (Milli-Q grade). The void elution volume t_0 was determined using formamide.

Reference Compound. The method requires a reference compound for which $\Delta_{OW}H$ is well established, that is, for which K_{OW} is accurately known within the temperature range of the experiments, preferably by methods such as the "shake flask", or "slow stirring" method. 1,3,5-trichlorobenzene was selected as a reference compound and the temperature-dependent K_{OW} values reported for this substance by Bahahur et al. (1998) for the range 5 °C to 55 °C (see Table 1) were employed. The $\Delta_{OW}H_{ref}$ is 18.2 kJ/mol.

Determination of the Parameters B. Capacity factors k' determined for seven CBzs (1,2-diCBz, 1,4-diCBz, 1,3,5-triCBz, 1,2,3,4-tetraCBz, 1,2,3,5-tetraCBz, penta-CBz, hexa-CBz) at six temperatures were regressed against ln K_{OW} as reported for these temperatures in Bahadur et al. (1998) to obtain values for the slope B in eq 1 at each of the experimental temperatures (see Table 1). The relationships were always linear with r^2 around 0.979 ± 0.002.

Results and Discussion

Determination of the Enthalpy of Octanol−Water Phase Transfer $\Delta_{OW}H$. For each substance ln k'/k'_{ref} was determined at several temperatures and regressed against ln K_{OWref}/B from Table 1. The relationship were always highly linear (r^2 of these regressions was typically higher than 0.97). Triplicate injections were performed at each temperature, and the k'/k'_{ref} ratios, which can be found in the Supporting Information, were always reproducible within 1%. The $\Delta_{OW}H$ values obtained using eq 6 are listed in Tables 2 and 3. The values for all compounds are between 13 and 32 kJ/mol confirming a relatively minor temperature dependence of the partitioning between water and octanol.

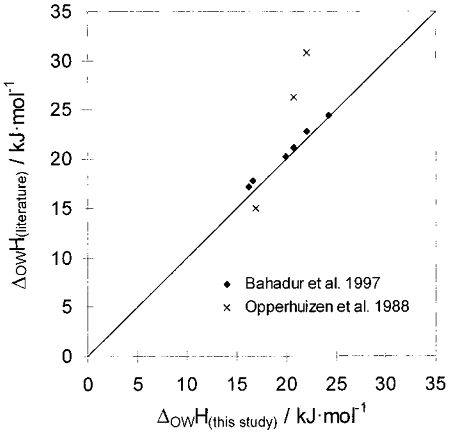

Figure 1. Comparison of the enthalpy of octanol to water phase transfer $\Delta_{OW}H$ for chlorobenzenes obtained in this study with those reported by Bahadur et al. (1997) and Opperhuizen et al. (1988).

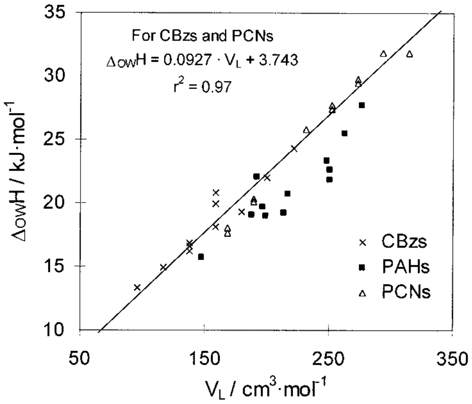

Figure 2. Relationship between the enthalpy of octanol−water phase transfer $\Delta_{OW}H$ and the liquid molar volume V_L for CBzs, PCNs, and PAHs.

The availability of data to evaluate these enthalpies of phase transfer is very limited. For the chlorinated benzenes it is possible to compare the $\Delta_{OW}H$ obtained in this study with those reported previously (Opperhuizen et al., 1988, Bahadur et al., 1997) (Figure 1). The HPLC estimation method gives results for $\Delta_{OW}H$ which are very close to, that is, within 2 kJ/mol of, those reported by Bahadur et al. (1997). This, however cannot be regarded as a truly independent test of the method, because the HPLC method relied on these data both for the reference compound and to derive the temperature-dependent parameters B. Although not sufficient, this agreement is a necessary criterion for the validity of the method. The agreement with the $\Delta_{OW}H$ reported by Opperhuizen et al. (1988) is poor, but this was expected as the results of the two previous studies (Opperhuizen et al., 1988, Bahadur et al., 1998) deviated considerably from each other, and the new data can thus only agree with one of them.

Figure 2 plots $\Delta_{OW}H$ against molar volume calculated using the Le Bas method. This method is based on the summation of atomic volumes and a subsequent adjustment of the volume decrease arising from ring formation (Reid et al., 1987). The data suggest a strong positive

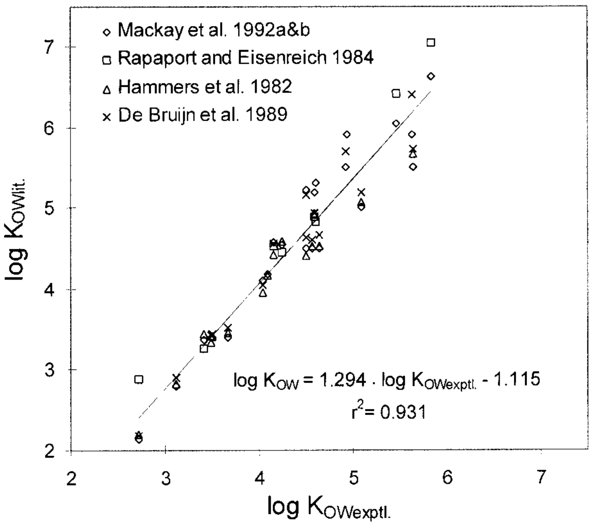

Figure 3. Regression between the uncalibrated log K_{OWexptl} values obtained from temperature-dependent capacity factors on a RP-HPLC column and log K_{OW} values reported by Hammers et al., 1982, Rapaport and Eisenreich, 1984, De Bruijn et al., 1989, and the selected value in Mackay et al., 1992a and b.

correlation between the molecular size of a chlorinated planar aromatic compound and its enthalpy of octanol–water phase transfer. Apparently, unsubstituted planar aromatic compounds have a lower $\Delta_{\mathrm{OW}}H$ than chlorinated benzenes and naphthalenes of the same molecular size.

Determining K_{OW} at 25 °C for Selected PCNs and PAHs. The temperature-dependent elution volumes on the RP-HPLC column can also be used to obtain estimates of log K_{OW} at one temperature. Using the ln k'/k'_{ref} versus ln K_{OWref}/B regression from above and eq 7, an uncalibrated K_{OWexptl} at 25 °C for all chemicals was obtained. This method of obtaining a K_{OW} is superior to directly using eq 1, because it makes use of the measurements at all temperatures and reduces extrapolation errors (Hamilton, 1980). As the RP-HPLC is an indirect method, it is preferable to perform a calibration to obtain reliable K_{OW} value.

A calibration using a regression between the HPLC derived $K_{\mathrm{OWexptl.}}$ and K_{OW} values determined by classical methods can eliminate small systematic errors which depend on the column packing used. This was accomplished by regressing log K_{OWexptl} for the 23 chemicals in Table 2 against literature values log $K_{\mathrm{OWlit.}}$ (Hammer et al., 1982; Rapaport and Eisenreich, 1984; De Bruijn et al., 1989; Mackay et al. 1992a, 1992b). Figure 3 shows this calibration plot and gives the respective regression equation. The same regression describes the behavior of CBzs, PCBs and PAHs, all of which are aromatic substances that lack polar functional groups. Whereas the relationship is very tight for intermediate K_{OW} values, it is less so for the higher range, possibly reflecting the higher uncertainty of high K_{OW} values from the literature. The fact that one calibration equation is sufficient to describe the relationship between log $K_{\mathrm{OWlit.}}$ and log K_{OWexptl} implies that all experimental compounds can be treated with one set of regression constants in eq 1, lending support for the use of that equation in the derivation of $\Delta_{\mathrm{OW}}H$ for these compounds. It also justifies the use of the calibration equation to derive K_{OW} values for other representatives of these compound classes as well as for the structurally related PCNs.

Using the log K_{OWexptl} and this regression (Figure 3), a log K_{OW} at 25 °C was estimated for 15 chemicals, namely the PCN congeners and selected PAHs. The results are given in Table 3. Log K_{OW} as a function of temperature can be calculated from $\Delta_{\mathrm{OW}}H$ and K_{OW} at a reference temperature T_{ref} using

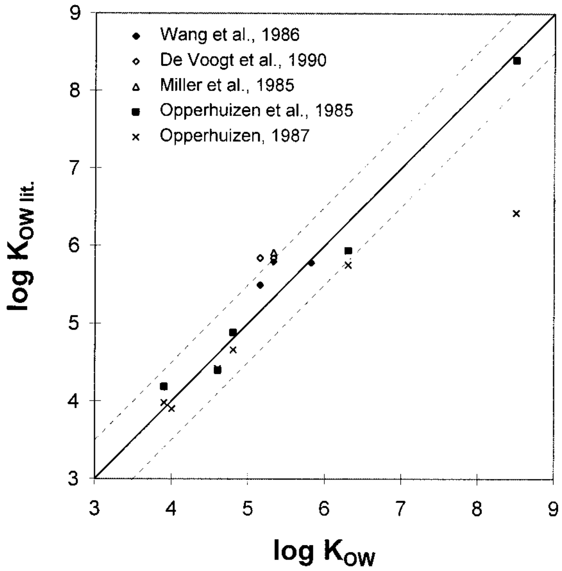

Figure 4. Comparison of the log K_{OW} for three PAHs and six PCNs measured in this study with those reported in the literature (compound identities and values given in Table 3).

$$\log K_{\mathrm{OW}}(T) = \log K_{\mathrm{OW}}(T_{\mathrm{ref}}) + \frac{\Delta_{\mathrm{OW}}H}{2.303R}\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right) \quad (8)$$

To facilitate this calculation, Table 3 also lists the parameters *A*, combining the terms referring to the reference temperature ($T_{\mathrm{ref}} = 25$ °C) in one expression; thus

$$\log K_{\mathrm{OW}} = A - \Delta_{\mathrm{OW}}H/(2.303RT) \quad (9)$$

For some of these 15 compounds, log K_{OW} had been reported previously (Table 3), and the values reported here tend to be within 0.5 log units of these literature values (Figure 4). An exception is octachloronaphthalene for which two widely different values had been reported before. Our value agrees well with the higher of these two values, which had been measured by the HPLC retention time technique (Opperhuizen et al., 1985).

In conclusion, we believe that this novel and rapid method to estimate $\Delta_{\mathrm{OW}}H$ is convenient and often sufficiently accurate and reliable, because the effect of temperature on K_{OW} is relatively minor, and would in most cases not justify the large effort involved in performing a traditional shake flask technique at several temperatures.

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Supporting Information Available:

A table showing the average and standard deviation of three determinations of k'/k'_{ref} of each substance at various temperatures. This material is available free of charge via the Internet at http://pubs.acs.org.

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