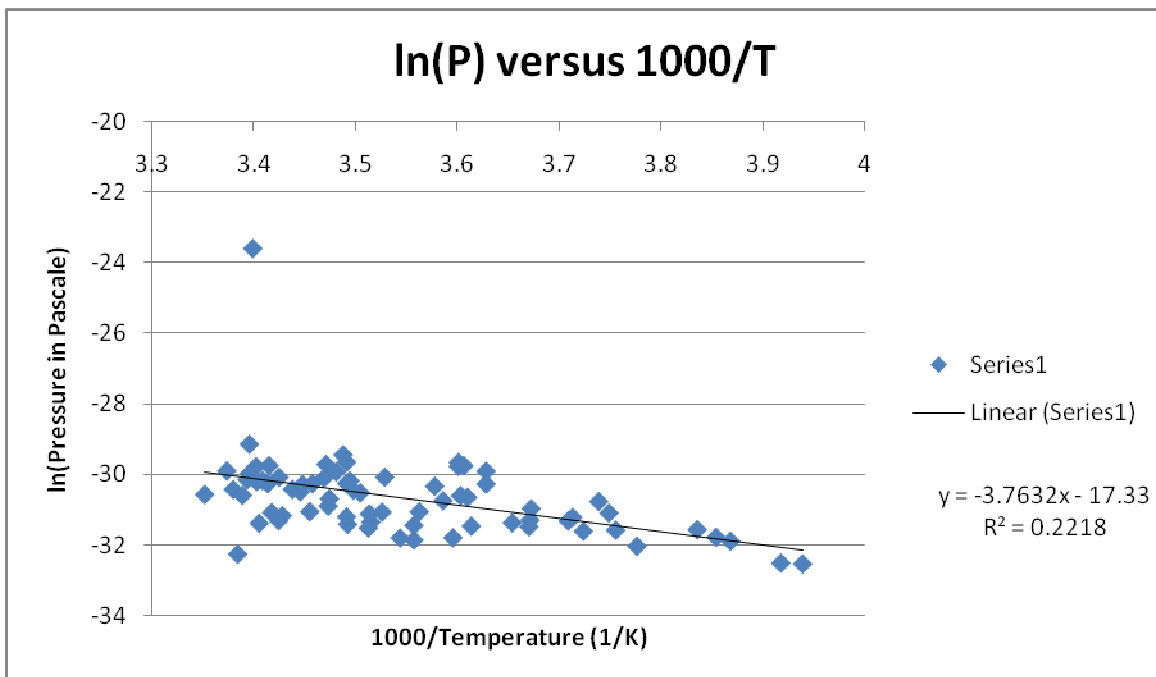


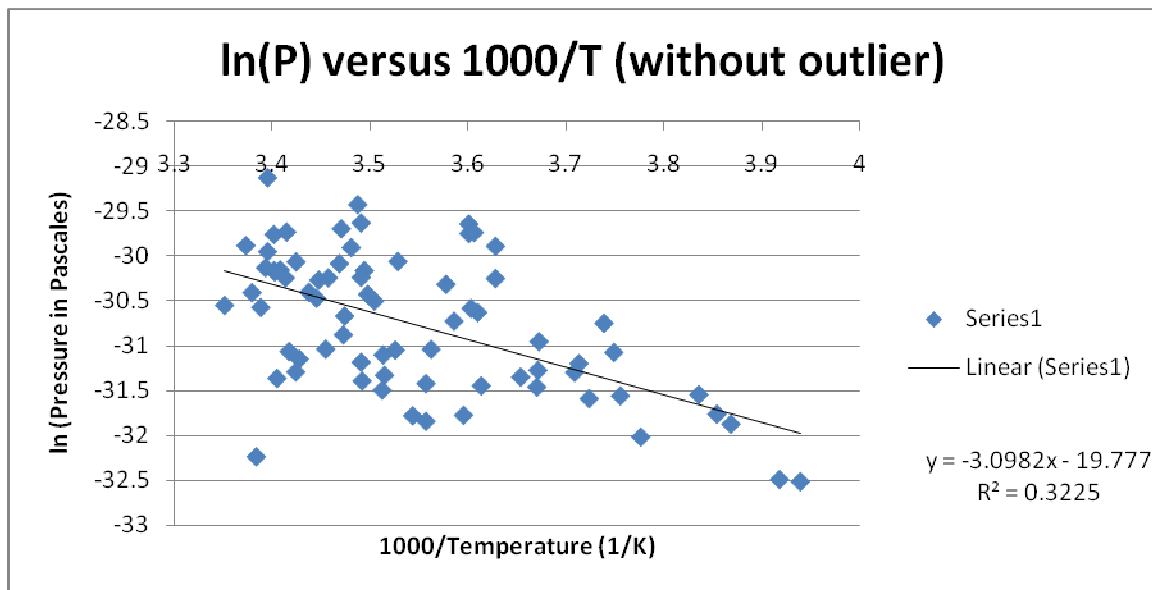
Regression of ln(P) and (1000/T)—with outlier

SUMMARY OUTPUT								
<i>Regression Statistics</i>								
Multiple R	0.470975							
R Square	0.221817							
Adjusted R Square	0.211009							
Standard Error	1.007024							
Observations	74							
ANOVA								
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>			
Regression	1	20.81256	20.81256	20.52322	2.29E-05			
Residual	72	73.01506	1.014098					
Total	73	93.82761						
	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	-17.3297	2.94623	-5.882	1.17E-07	-23.2029	11.4565	23.2029	11.4565
X Variable 1	-3.76323	0.830687	4.53026	2.29E-05	-5.41917	2.10728	5.41917	2.10728



Regression of ln(P) and (1000/T)—without outlier—1<sup>st</sup> data entry, which is way out there!

SUMMARY OUTPUT								
<i>Regression Statistics</i>								
Multiple R	0.567852							
R Square	0.322456							
Adjusted R Square	0.312913							
Standard Error	0.641388							
Observations	73							
ANOVA								
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>			
Regression	1	13.90056	13.90056	33.79018	1.61E-07			
Residual	71	29.20789	0.411379					
Total	72	43.10844						
	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	-19.7772	1.891425	10.4562	5.11E-16	-23.5486	16.0058	23.5486	16.0058
X Variable 1	-3.09822	0.532987	5.81293	1.61E-07	-4.16096	2.03547	4.16096	2.03547



WRITTEN SUMMARY:

Congener 56 (+60): 2,3,3',4-tetrachlorobiphenyl (coeluting with 2,3,4,4'-tetrachlorobiphenyl)  
CAS #: 033025-41-1 Name: 2,3,4,4'-TETRACHLOROBIPHENYL

• **R-value and Significance of F-statistic:** The r-values are less than 0.7 ( $r = 0.47$  with the outlier, 0.56 without the outlier) indicating a weak linear correlation. The F-statistic significance is less than  $\alpha = 0.05$  or 0.01 (F-stat. sig =  $2.29 \times 10^{-5}$  with the outlier,  $1.61 \times 10^{-7}$  without it), so there is a linear relationship at the 95% and 99% confidence level.

• **Slope and  $\Delta H$  (kJ/ mol):** The  $\Delta H$  value obtained was low, less than 50 kJ/ mol (31.8 kJ/ mol with the outlier, 25.8 kJ/ mol without the outlier), which indicates that this congener is fairly volatile and the source of this congener is not local.

• **HLC data:** HLC =  $1.25 \times 10^{-5}$  atm-m<sup>3</sup>/ mole (citation: <http://www.syrres.com/esc/physdemo.htm>) The group showed an inverse relationship between the  $\Delta H$  and HLC values.