

A Simple Structure-Based Calculator for Estimating Vapor Pressure

Kirk A. Simmons*

Discovery Research Department, Agricultural Products Group, FMC Corporation, P.O. Box 8,
Princeton, New Jersey 08543

The development of an estimator for vapor pressure based upon organic functional groups is described. This vapor pressure calculator permits prediction of vapor pressure for a wide range of structural classes. The statistical quality of the derived coefficients is presented as well as the quality of the prediction of the training set of compounds. The calculator is then used to predict the vapor pressure of recently introduced agrochemicals to illustrate its performance. The significance of this calculator is that the agrochemical scientist can readily estimate the effects on vapor pressure of altering specific structural features of a molecule.

Keywords: Volatility; vapor pressure; regression; prediction; physical properties

INTRODUCTION

The physical properties of a compound greatly influence its behavior in the environment (Baum, 1998; Domine et al., 1992; Hartley and Graham-Bryce, 1980). Changes in physical properties such as lipophilicity ($\log P$) or volatility ($\log V_p$) can, for example, affect whether a compound will move in soil and perhaps be leached to groundwater (Grover, 1988; Suntio et al., 1988). In the discovery of both preemergent herbicides and soil-applied insecticides, the overall performance of any given molecule is governed by its lipophilicity and volatility (Figure 1) (Simmons et al., 1992a,b).

During the synthesis of analogues around a lead structure, a compound must ultimately be produced that not only optimally binds the target receptor or enzyme but also possesses sufficient bioavailability and stability to reach that biological target in the organism in its natural environment. An earlier assessment of bioavailability of a chemical series in a discovery program is expected to improve the overall program success by producing compounds with the required biological activity in the target environment.

Vapor pressure can be experimentally determined (Hamilton, 1980; Kim et al., 1984; Anonymous, 1950) by techniques of various complexity, and measurement should be preferred to prediction whenever possible. However, our interest is focused at the stages of agrochemical discovery when the chemist is making structural modifications to a molecule with the goal of improving bioavailability of an analogue series. The scientist is here faced with forecasting bioavailability of an, as yet, unsynthesized compound. Since such bioavailability is a function of physical properties, predicting these properties would be expected to facilitate the process of predictably altering bioavailability in a chemical series. Models for predicting vapor pressure from calculated molecular descriptors have been reported (Katritzky et al., 1998). Molecular descriptor-based models, however, require computation of these descriptors in order to predict the vapor pressure of each

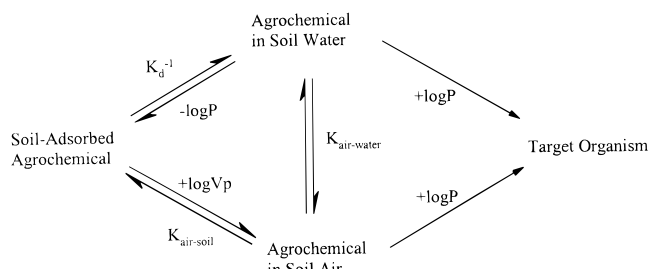


Figure 1. Equilibrium distribution of an agrochemical in soil.

Table 1. Examples of Isomer Effect on Boiling Point

compound	bp (°C)	compound	bp (°C)
2-fluorophenol	173	4-isopropylaniline	228
4-fluorophenol	186	2-ethylphenol	197
2-isopropylaniline	215	4-ethylphenol	219

new structure. Models for predicting boiling points from group contributions have also been reported (Stein and Brown, 1994). While group contribution-based property predictors are easier to use in forecasting new structures, most models of environmental movement of agrochemicals are based on vapor pressure and not directly on boiling point (Domine et al., 1992; Suntio et al., 1988).

A simple calculator has been constructed that has proven useful in predicting vapor pressure of compounds based upon their structure and melting point. Desirable features of this calculator are easy implementation and the capability to estimate vapor pressure across varied structural classes, and because it is based upon group contributions, it has the advantage of simplicity and generality. This paper describes the development of this calculator based upon standard organic functional group contributions.

MATERIALS AND METHODS

A search of the literature provided several secondary sources for vapor pressure measurements on which to build this calculator (Boublik et al., 1973; Jordan, 1954; Montgomery, 1993; Ohe, 1976; Weast, 1968; Stull, 1947). These data were used without verifying their quality. Although these data are reported and analyzed in units of mmHg, they could be readily converted to Pascals (133.3 mmHg = 1 Pascal). The available

* To whom correspondence should be addressed (e-mail, kirk_simmons@fmc.com; fax, 609-951-3330).

Table 2. Regression-Derived Functional Group Contributions to Clog V_p

fragment description	aliphatic			aromatic		
	coefficient	error	<i>p</i> -tail	coefficient	error	<i>p</i> -tail
intercept	4.42	0.040	<0.0001	4.42	0.040	<0.0001
(mp - 25)/100	-1.56	0.077	<0.0001	-1.56	0.077	<0.0001
intramolecular H-bonding	0.73	0.052	<0.0001	0.73	0.052	<0.0001
block intermolecular H-bonding	0.53	0.073	<0.0001	0.53	0.073	<0.0001
X-CH ₃	-0.28	0.014	<0.0001	-0.34	0.033	<0.0001
X-CH ₂ R	-0.45	0.004	<0.0001	-0.26	0.031	<0.0001
X-CHR ₂	-0.39	0.016	<0.0001	-0.19	0.056	0.0006
X-CR ₃	-0.38	0.035	<0.0001	-0.18	0.088	0.0387
X-CH _(2-n) R _n Ar				0.05	0.135	0.6941
=CH-				-0.46	0.008	<0.0001
=CX-	-0.63	0.025	<0.0001	-0.63	0.025	<0.0001
=N-				-0.94	0.041	<0.0001
terminal alkene/alkyne	-0.65	0.033	<0.0001	-0.65	0.033	<0.0001
internal alkene/alkyne	-1.00	0.030	<0.0001	-1.00	0.030	<0.0001
X ₂ C=C=CX ₂	-1.21	0.183	<0.0001	-1.21	0.183	<0.0001
X(R)C=CR ₂	-0.25	0.088	0.0044	-0.25	0.088	0.0044
X-CHO	-1.21	0.085	<0.0001	-1.40	0.126	<0.0001
X-COR	-1.63	0.088	<0.0001	-1.46	0.088	<0.0001
X-COAr	-1.46	0.088	<0.0001	-0.71	0.118	<0.0001
X(R)C=NOR	-1.84	0.221	<0.0001			
X-CO ₂ H	-3.67	0.053	<0.0001	-4.69	0.133	<0.0001
X-CO ₂ R	-1.43	0.026	<0.0001	-1.19	0.080	<0.0001
X-NHCO ₂ Ar	-3.46	0.114	<0.0001	-3.46	0.114	<0.0001
X-OCO ₂ R	-1.92		<i>n</i> = 1			
X-OR	-0.43	0.033	<0.0001	-0.70	0.045	<0.0001
X-OAr	-0.70	0.045	<0.0001	-0.33		<i>n</i> = 1
-O- in a furan				-0.72	0.130	<0.0001
X-SR	-1.29	0.062	<0.0001	-0.83	0.130	<0.0001
X-SAr	-0.83	0.130	<0.0001	-0.98	0.151	<0.0001
-S- in a thiophene				-0.54	0.094	<0.0001
X-SOR	-3.21	0.224	<0.0001			
X-SO ₂ R	-3.05	0.269	<0.0001	-2.72		<i>n</i> = 1
X-SO ₂ Ar	-2.72	<i>n</i> = 1		-2.02	0.369	<0.0001
X-OSO ₂ R	-2.50	<i>n</i> = 1				
X-OSO ₃ R	-3.63	<i>n</i> = 1				
X-SH	-1.16	0.085	<0.0001	-1.20	0.363	0.001
X-OH 1o	-2.09	0.048	<0.0001	-1.79	0.058	<0.0001
R-OH 2o	-1.58	0.065	<0.0001			
R-OH 3o	-1.52	0.103	<0.0001			
X-F	0.07	0.049	0.1321	0.21	0.034	<0.0001
X-Cl	-0.79	0.026	<0.0001	-0.53	0.029	<0.0001
X-Br	-1.18	0.039	<0.0001	-0.84	0.074	<0.0001
X-I	-1.71	0.093	<0.0001	-1.24	0.213	<0.0001
X-CF ₂ R	-0.33	0.023	<0.0001			
X-CCl ₂ R	-1.53	0.076	<0.0001			
X-CBr ₂ R	-2.70	0.117	<0.0001			
X-CF ₃	-0.20	0.047	<0.0001	0.32	0.109	0.0029
X-CCl ₃	-1.89	0.095	<0.0001	-2.63	0.216	<0.0001
X-CBr ₃	-3.47	0.261	<0.0001			
X-NO ₂	-2.51	0.165	<0.0001	-1.45	0.057	<0.0001
X-CN	-1.88	0.079	<0.0001	-1.36	0.138	<0.0001
X-NH ₂	-0.80	0.103	<0.0001	-1.93	0.073	<0.0001
X-NHNH ₂				-2.92	0.257	<0.0001
X(R)NNH ₂	-1.71	0.258	<0.0001	-1.71	0.258	<0.0001
XNHNHR	-2.00		<i>n</i> = 1			
X-NHR	-0.86	0.130	<0.0001	-1.00	0.078	<0.0001
X-NHAr	-1.00	0.078	<0.0001	-1.96	0.262	<0.0001
-NH- in an azole				-1.78	0.211	<0.0001
XNHOR	-1.27		<i>n</i> = 1			
X(R)NOR	-0.77		<i>n</i> = 1			
X(R)NOH	-2.52		<i>n</i> = 1			
X-N(-)	-0.50	0.075	<0.0001	-0.50	0.075	<0.0001
SiR ₄	-0.57	0.118	<0.0001			
Si(OR) ₄	-1.19	0.364	0.0011			
X-SCN	-3.06	0.363	<0.0001			
X-NCS	-2.73	0.183	<0.0001	-2.22	0.363	<0.0001
X-NCO				-1.16	0.130	<0.0001
X-CONH ₂	-5.18	0.258	<0.0001			
X-NHCOR	-4.68	0.165	<0.0001	-4.68	0.165	<0.0001
X-NHCO ₂ R	-4.36	0.132	<0.0001	-4.36	0.132	<0.0001
X-OCONH ₂	-4.14	0.211	<0.0001			
X-CONR ₂	-2.46	0.086	<0.0001	-2.46	0.086	<0.0001
X-CONR ₂ Ar	-1.12	0.192	<0.0001	-1.12	0.192	<0.0001
X-OP(=O)(OR) ₂	-2.67	0.111	<0.0001			
X-SP(=S)(OR) ₂	-3.40	0.097	<0.0001			

Table 2. (Continued)

fragment description	aliphatic			aromatic		
	coefficient	error	<i>p</i> -tail	coefficient	error	<i>p</i> -tail
X-OP(=S)(OR) ₂	-3.16	0.184	<0.0001	-2.17	0.120	<0.0001
X-SP(=O)(OR) ₂	-3.79	0.204	<0.0001	-3.79	0.204	<0.0001
X(R)C=NOC(=O)NHR	-5.07	0.192	<0.0001			
X-NHCONR ₂	-6.47	0.120	<0.0001	-6.47	0.120	<0.0001
X-SCONR ₂	-3.01	0.119	<0.0001			
X-NHCOAr				-2.80	0.270	<0.0001
X-N=NAr				-0.97	<i>n</i> = 1	
X-NHCOC(Me) ₂ CH ₂ SAr	-4.83	0.138	<0.0001	-4.83	0.138	<0.0001
X-NHCON(R)(OR)	-4.88	0.216	<0.0001	-4.88	0.216	<0.0001
X-N=CH-NR ₂	-3.28	0.264	<0.0001	-3.28	0.264	<0.0001

structures were coded by counting the number of times each organic functional group was present in the structure. The contribution of each functional group to vapor pressure was determined from the regression coefficients derived from multiple linear regression (Dixon, 1988).

Building the calculator started with compounds representing alkanes, alkenes, and alkynes. Then compounds were included which contained the following organic functional groups: ester, ketone, ether, thioether, alcohol, thiol, halide, nitro, cyano, aldehyde, amine, silicon, carboxylic acid, carboxamide, sulfoxide, sulfone, carbamate, phosphate, and thiophosphate. Once the data for these functional groups were exhausted, structures were added which exemplified agrochemicals. Generally compounds which contained similar functional groups were added to the data set in stages. At each stage, linear regression was reapplied and the resulting coefficients were examined. If, in the process of adding new structures, the variance about any of the regression-derived coefficients significantly increased, the input file was examined for possible structure coding errors, which were then corrected. If no errors had been made in coding the structures, the new cases were examined as a group. If they were consistently poorly predicted, the structural features were recoded with a more complex functional group that included more of the base structure. Our rule was to always code the more complex functional group and avoid building it from simpler ones. For example, esters (-CO₂-) were coded uniquely and not as being made of a carbonyl (-C=O) and ether (-O-). Functional groups attached to an aromatic ring system were coded separately from those attached to an aliphatic system, where sufficient examples of each were available. Where there were insufficient examples, no distinctions were made between these environments and a single fragment contribution was derived.

During the course of development, compounds that contained functional groups capable of forming hydrogen bonds began to show a pattern. If a compound could form an intramolecular hydrogen bond, it was always more volatile than an isomer that could not (i.e., compare 2-fluorophenol vs 4-fluorophenol in Table 1). Intramolecular hydrogen bonding was coded as a fragment that reflected the ability of a five- or six-membered hydrogen-bonded ring to form within the structure. It was also noted that in compounds with functional groups capable of forming hydrogen bonds and also substituted in the adjacent position by a bulky group, vapor pressure was greater than expected (i.e., compare 2-ethyl and 2-isopropyl isomers vs 4-ethyl and 4-isopropyl isomers in Table 1). A fragment specifically coded this situation as well. Our coding philosophy is similar to that used in estimating normal boiling points using group contributions (Stein and Brown, 1994).

Crystalline compounds exhibit a lower vapor pressure than liquids as their crystal lattice must be disrupted before the material can vaporize. This situation was coded by including the melting point as one of the independent variables, using the following transformation suggested by Yalkowsky's modeling of water solubility (Yalkowsky and Morozowich, 1980):

$$\text{mp correction} = (\text{mp } ^\circ\text{C} - 25)/100$$

If a compound was a liquid at 25 °C, then 25 °C was used as its melting point. One note of caution is appropriate here. The

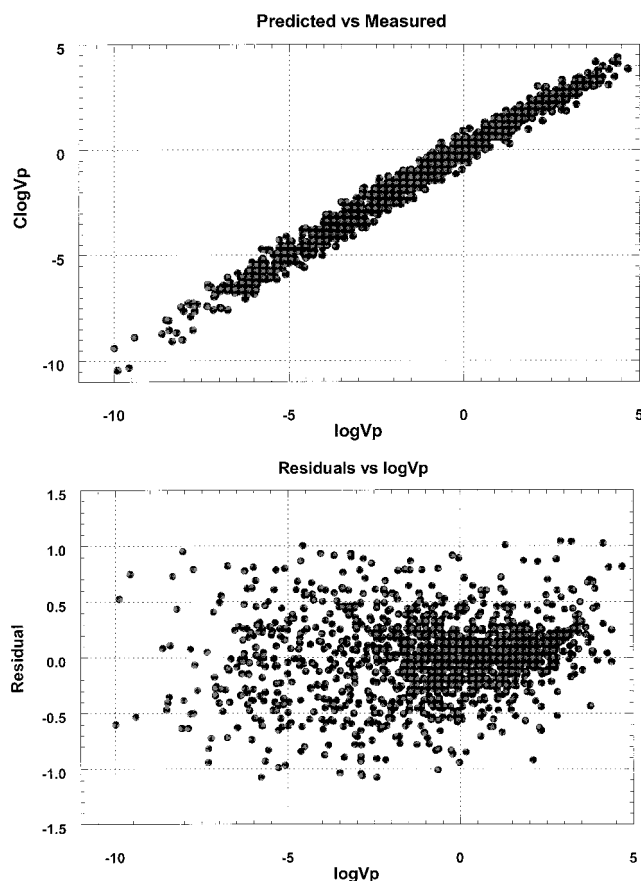


Figure 2. Predicted versus measured for the training set.

vapor pressures of solids are often measured above their melting point and then extrapolated to 25 °C. Vapor pressures measured in this fashion would overestimate the volatility of the solid at 25 °C. It was not always obvious if reported vapor pressures were determined at 25 °C or extrapolated to 25 °C, and this is one source of possible error.

RESULTS AND DISCUSSION

Once all of the available data were entered and analyzed, compounds whose predicted vapor pressure differed from the reported vapor pressure by more than 3 standard deviations were removed in the derivation of the final fragment constants. Our final data set consisted of 1410 compounds described by 94 functional groups. The final regression model on which the fragment constants in Table 2 were derived is expressed in eq 1:

$$\text{Clog } V_p = \sum a_i^* f_i - 1.56 * (\text{mp} - 25)/100 + 4.42 \quad (1)$$

$$n = 1410 \quad s = 0.36 \quad r^2 = 0.98 \quad F = 650 \quad (p\text{-tail} < 0.001)$$

Table 3. Secondary Functional Group Contributions to Clog V_p ^a

fragment description	aliphatic			aromatic		
	coefficient	error	<i>p</i> -tail	coefficient	error	<i>p</i> -tail
X-CO ₂ CH(CN)Ar	-2.89	0.26	<i>n</i> = 3			
X(R)-NC(=NNO ₂)NHR	-5.82		<i>n</i> = 1			
X-N(OR)C(=O)R	-2.97		<i>n</i> = 1			
X-SP(=O)(OR)(NHCOR)	-9.27		<i>n</i> = 1			
X-N*C(=S)N(R)N=C*R				-3.11	0.75	<i>n</i> = 5
X-N*C(=O)N(R)C(R)=C(R)C*(=O)				-2.70	0.34	<i>n</i> = 3
X-SO ₂ NHCONHAr				-3.07	0.80	<i>n</i> = 4
X-CONHCONHAr				-1.29		<i>n</i> = 1
X-N*C(=O)N(R)C(R)=N*				-4.04	1.07	<i>n</i> = 2
X(R)-C=NN(R)C(=O)N(Ar)CO ₂ R				-1.01		<i>n</i> = 1

^a An asterisk (*) denotes the points of attachment for a cyclic system.

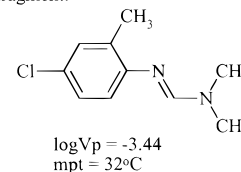
where a_i is the regression coefficient for the i th fragment, f_i is the number of times the i th fragment occurs in the structure, n is the number of cases, s is the standard error of the regression, r^2 is the explained variance, and F is the appropriate f -test statistic. The plot of predicted vapor pressure versus measured vapor pressure for the training set is presented in Figure 2. The quality of this model is comparable to others reported which are based on calculated molecular descriptors ($r^2 = 0.95$, $s = 0.33$) (Katritzky et al., 1998). However, models based upon molecular descriptors require recalculation of those descriptors to estimate the effect of, for example, modifying a methyl ester to an isopropyl ester. And while the final estimated property values are likely equally accurate by either method, a group contribution-based method is easier to implement for a series of "what-if" type analyses, which are common in later stages of optimization of a chemical series.

The regression results in eq 1 indicate an upper limit for vapor pressure of $10^{4.42}$ mmHg at 25 °C. The most volatile substances are hydrogen and helium, and their vapor pressures have been reported (Weast, 1968) to be 760 mmHg at -252.5 and -268.6 °C, respectively. Assuming ideal gas behavior ($P_1 T_2 = P_2 T_1$) these data extrapolate to log V_p values at 25 °C of 4.0 and 4.7, respectively, in excellent agreement with the regression constant of 4.42.

The convention used in Table 2 is that X in the fragment description denotes the point of attachment for the functional group. "R" and "Ar" denotes further substitution within polyvalent fragments for aliphatic and aromatic attachments, respectively. Functional group contributions to vapor pressure are listed under the column headings "aliphatic" and "aromatic". When the fragment vapor pressure values are identical under both columns, they were derived across both aliphatic and aromatic examples that had been combined due to limited data. Analysis of further examples may indicate that these fragment contributions differ between aromatic and aliphatic environments, but the current data were insufficient to make this distinction. Once the primary fragment constants were derived, secondary fragments were defined. Secondary fragments in Table 3 carry only vapor pressure contribution and error estimates and have no t -value since they were not derived from regression analysis. The number of cases for each functional group is listed. Secondary fragment values were derived for those functional groups represented by a limited number of examples and were assigned as the difference between the measured and predicted vapor pressure when all of the primary

fragment contributions were taken into account. See the following example for clarification.

Assigning a secondary fragment:



Occurrences	Primary Fragment	Secondary Fragment	Contribution ClogVp	
1	-Cl		-0.53	
3	=CX-		-1.89	
3	=CH-		-1.38	
2	-CH ₃		-0.56	
1	-CH ₃		-0.34	
1	Constant		4.42	
(32-25)/100	mpt		-0.11	
1		-N=CH-NR ₂	(-3.05)	Assigned 2 ^{ndary} value
			-3.44	Measured logVp

Several general observations are worth noting. The first is that functional groups attached to an aromatic system tend to impart more volatility than when attached to an aliphatic system. There are certainly exceptions within Table 1, but this general pattern may allow for the estimation of aromatic functional group contributions from aliphatic cases, and vice versa. This trend is also evident with boiling point estimation from group contributions (Stein and Brown, 1994). The second observation is that estimating a complex functional group by building it up from smaller defined fragments often produces poorer estimates. For example, the α -cyanoester functional group of the pyrethroid insecticides has a vapor pressure group contribution of -2.89 ± 0.26 when coded as a single unit but a value of -3.70 if estimated by combining smaller defined functional groups ($-\text{CO}_2-$ + $-\text{CH}-$ + CN). This would suggest that the earlier choice, always to code the larger functional group, was a wise one.

Validation of Model. Predicting the vapor pressure of various agrochemicals, not used in the development of the calculator, offers an example of the utility of this simple vapor pressure calculator. These predictions are summarized in Table 4 for the compounds listed in Figure 3 (Ammermann et al., 1992; Deege et al., 1995; Hanai et al., 1993; Hartwig et al., 1992; Longhurst et al., 1992; Luscombe et al., 1995; Matsuo, 1998; Meister, 1995; Miura et al., 1993; Neumann et al., 1992; Prosch et al., 1997; Russell et al., 1992; Snel et al., 1995; Suntio et al., 1988; Tomlin, 1997). A plot of the predicted versus measured vapor pressure values is presented in Figure 4.

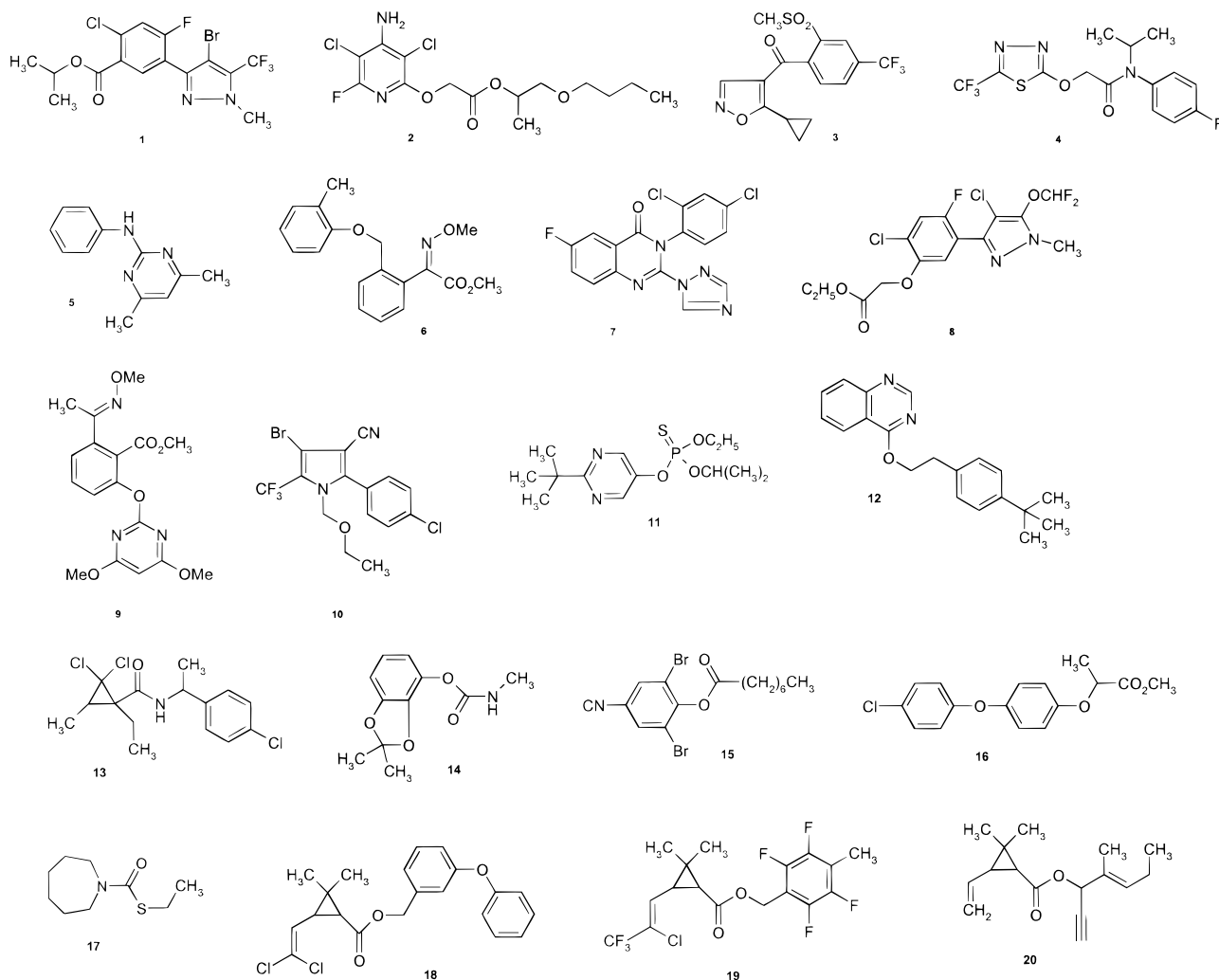


Figure 3. Structures for compounds listed in Table 4.

Table 4. Predictions Using Vapor Pressure Calculator

agrochemical	structure	log V_p (mmHg)			mp ($^{\circ}$ C)
		measd	pred	diff	
isopropazol	1	-7.2	-7.2	0.0	81
fluroxypyr, butoxy-1-methylethyl ester	2	-7.4	-7.7	-0.3	liquid
RPA 201772	3	-8.1	-8.4	-0.3	140
BAY FOE 5043	4	-6.2	-7.2	-1.0	77
pyrimethanil	5	-4.8	-6.0	-1.2	96
kresoxim-methyl	6	-7.6	-8.2	-0.6	102
fluquinazone	7	-10.3	-11.6	-1.3	193
ET-751	8	-9.4	-9.4	0.0	127
KIH-6127	9	-7.3	-9.9	-2.3	105
AC-303630	10	-7.0	-6.9	0.1	100
MAT 7484	11	-4.5	-4.6	-0.1	liquid
fenazaquin	12	-5.9	-7.2	-1.3	liquid
KTU 3616	13	-8.7	-9.6	-0.9	149
bendiocarb	14	-5.3	-5.9	-0.6	130
bromoxynil octanoate	15	-5.3	-5.4	-0.1	46
diclofop-methyl	16	-5.6	-5.4	0.2	41
molinat	17	-2.3	-2.0	0.3	liquid
permethrin	18	-7.4	-7.4	0.0	39
tefluthrin	19	-4.4	-4.6	-0.2	liquid
empenthrin	20	-3.0	-2.4	-0.6	liquid
average difference				0.57	

The results using this organic functional group-based vapor pressure calculator are quite encouraging with an average error of prediction of only 0.57. Of course for new analogues one needs an estimate of the melting point. Given the small coefficient (0.0156) for the

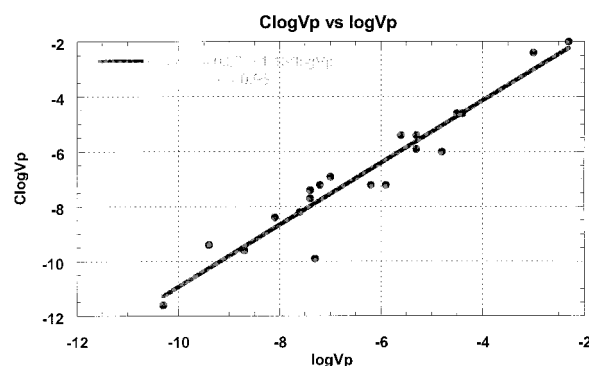


Figure 4. Measured (log V_p) versus predicted (Clog V_p) for 20 agrochemicals.

melting point term in eq 1, an approximate melting point (within ± 32 $^{\circ}$ C) is all that is required to predict vapor pressure within 0.5 log unit. One could estimate the melting point from the most similar known analogue or from appropriate methods in the literature (Dearden, 1991). We have found estimating the melting point of a new analogue in a series as the running average of all previous analogues to be quite satisfactory.

CONCLUSION

The ability to predict vapor pressures within 4-fold ($10^{0.57}$) across a vapor pressure range of 10^8 mmHg

using only structure and melting point should prove useful in the design and optimization of soil-applied agrochemicals. Predictions of vapor pressure within a chemical analogue series would likely be even more accurate, especially if the vapor pressure of several analogues was measured and used to derive a vapor pressure contribution of the largest common substructure. The pesticide scientist would be able to reliably estimate the effects of structural modifications on vapor pressure within a chemical series. This calculator has been incorporated into a Microsoft Excel spreadsheet allowing for easy "what-if" type analyses of vapor pressure across possible analogues for synthesis.

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