SMILES	C=Cc1cnccn1			C_w=	
Compound No.	19959			C_g=	
Compound Name	**2-Vinylpyrazine**			**log Kw=**	
Molecular Formula	C6H6N2			P + L, count:	15
Molecular weight	106.1300	**WS (mg/L)=**			
CAS No	4177-16-6	**VP (mm Hg)=**		**P+L, sd:**	**0.037**
ACD/n20 =	1.568				
E =	0.909			Weight:	1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)		
	0.412		0.66	0.58	**P+L, sd(W):**	**0.037**

UNIX	SMART			PA		
0.85		logKw	4.386		P, count:	3
0.84		R (**E**)=	0.770	**0.77**		
0.00		Pi (**S**)=	0.900	**0.83**	**P, sd:**	**0.057**
0.60		Alpha (**A**) =	**0.000**	**0.00**		
3.89		Beta (**B**)=	0.710	**0.55**	L, count:	12
		LogL16 (**L**) =	3.881	**3.886**		
		Vx (**V**)=	0.8730		**L, sd:**	**0.035**

LogPcalc	LogPobs
1.475	1.431

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	LogPcalc	LogPcalc	LogPobs	(Po-Pc)^2	
	Octanol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	P	Octanol (wet)	0.445	0.445	0.412	0.001	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.442	-0.442	-0.504	0.004	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.423	4.423	4.386	0.001	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2
MHA unpub.	Octanol/Wet/March 98	-0.198	0.002	0.709	3.519	1.429	0.858	0.000	L	Octanol/Wet/March 98	4.786	4.786	4.798	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.881	3.881	3.881	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.422	4.422	4.386	0.001
JAFC (2002) 50(5)	BPX-5	0.411	0.000	1.247	1.297	0.169	2.033	0.000	RI/100	BPX-5	9.544	9.544	9.540	0.000
JAFC (2001) 49(9)	4315-4323	1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100		9.451	9.451	9.470	0.000
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	9.392	9.392	9.460	0.005
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	9.472	9.472	9.470	0.000
JAFC (2002) 50(8)	CP-Sil-5CB	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100	CP-Sil-5CB	9.100	9.100	9.070	0.001
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	9.045	9.045	9.010	0.001
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	9.066	9.066	9.010	0.003
JAFC (2001) 49(3)	HP-Wax	-1.473	1.389	7.264	11.276	0.000	2.192	0.000	RI/100	HP-Wax	14.642	14.642	14.670	0.001
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	9.498	9.498	9.470	0.001