SMILES	c1c(ncc(n1)CC)CC	19910.000		C_w=
Compound No.	19910			C_g=
Compound Name	**2,5-Diethylpyrazine**			**log Kw=**
Molecular Formula	C8H12N2			P + L, count: 10
Molecular weight	136.1900	**WS (mg/L)=**		
CAS No	13238-84-1	**VP (mm Hg)=**		**P+L, sd: 0.028**
ACD/n20 =	1.498			
E =	0.644			Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
	1.744		1.79	1.70	**P+L, sd(W): 0.028**

UNIX	SMART			PA	
0.73	0.620	logKw	3.665		P, count: 3
0.78		R (**E**)=	0.620	0.67	
0.00	0.00	Pi (**S**)=	0.730	0.71	**P, sd: 0.033**
0.58		Alpha (**A**) =	0.000	0.00	
4.98		Beta (**B**)=	0.720	0.50	L, count: 7
		LogL16 (**L**) =	4.743	4.912	
		Vx (**V**)=	1.1978		**L, sd: 0.029**

LogPcalc	LogPobs
2.179	2.162

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)	1.744	1.744	1.744	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.124	1.124	1.078	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.669	3.669	3.665	0.000

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	5.419	5.419	5.409	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.743	4.743	4.743	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.697	3.697	3.665	0.001
JAFC (2000) 48(6)	DB-1	0.643	0.000	0.730	0.903	0.000	2.007	0.000	RI/100	DB-1	10.694	10.694	10.740	0.002
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	10.942	10.942	10.910	0.001
JAFC (2001) 49(9)	4315-4323	1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100		10.917	10.917	10.890	0.001
J Sci Food Agric (2	HP-Wax	-0.817	1.823	6.556	10.730	0.000	2.073	0.000	RI/100	HP-Wax	14.931	14.931	14.920	0.000