SMILES	CCc1cnc(cn1)C		C_w= 0.000
Compound No.	19915		C_g= 0.000
Compound Name	**2-Methyl-5-ethylpyrazine**		**log Kw=** #DIV/0!
Molecular Formula	C7H10N2		P + L, count: 13
Molecular weight	122.1678	**WS (mg/L)=**	
CAS No	13360-64-0	**VP (mm Hg)=**	**P+L, sd: 0.080**
S-A/n20 =	1.502-1505		
E =			Weight: 1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	1.215		1.30	1.17	**P+L, sd(W): 0.080**

UNIX	**SMART**			**PA**	
0.73	0.626	logKw	3.826		P, count: 3
0.78		R (**E**)=	**0.660**	**0.67**	
0.00	0.00	Pi (**S**)=	0.740	**0.71**	**P, sd: 0.031**
0.58		Alpha (**A**) =	**0.000**	**0.00**	
4.48		Beta (**B**)=	0.720	**0.50**	L, count: 10
		LogL16 (**L**) =	4.295	**4.417**	
		Vx (**V**)=	1.0569		**L, sd: 0.092**

LogPcalc	LogPobs
1.856	1.837

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)	1.219	1.219	1.215	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.510	0.510	0.469	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.840	3.840	3.826	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	5.042	5.042	5.041	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.853	3.853	3.826	0.001
JAFC (1999) 47(4)	BPX5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX5	10.200	10.200	10.100	0.010
JAFC (2002) 50(8)	CP-SIL5-CB	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100	CP-SIL5-CB	9.852	9.852	9.730	0.015
JAFC (1981) 29(6)	SE-30	0.492	-0.342	1.287	1.788	-0.431	2.024	0.000	RI/100	SE-30	9.601	9.601	9.790	0.036
JAFC (1984) 32(5)	1013	0.601	-0.257	0.942	1.309	0.000	1.996	0.000	RI/100		9.701	9.701	9.720	0.000
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	9.797	9.797	9.700	0.009
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	9.726	9.726	9.750	0.001
JAFC (2001) 49(4)	BPX5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX5	10.062	10.062	10.060	0.000
JCA (2000) 905 23	CP-SIL5-CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL5-CB	10.015	10.015	10.080	0.004