SMILES	CCc1nc(C)cnc1		C_w= 0.000
Compound No.	19916		C_g= 0.000
Compound Name	**2-Methyl-6-ethylpyrazine**		**log Kw=** #DIV/0!
Molecular Formula	C7H10N2		P + L, count: 13
Molecular weight	122.1678	**WS (mg/L)=**	
CAS No	13925-03-6	**VP (mm Hg)=**	**P+L, sd: 0.066**
ACD/n20 =	1.500		
E =			Weight: 1.00

P*	ClogP	logP(MD)	logP(PA)	logP(ACD)	
	1.215		1.30	1.17	**P+L, sd(W): 0.066**

UNIX	SMART			PA	
0.73	0.629	logKw	3.816		P, count: 3
0.78		R (**E**)=	0.660	0.67	
0.00	0.00	Pi (**S**)=	0.740	0.71	**P, sd: 0.043**
0.58		Alpha (**A**) =	0.000	0.00	
4.48		Beta (**B**)=	0.720	0.50	L, count: 10
		LogL16 (**L**) =	4.271	4.417	
		Vx (**V**)=	1.0569		**L, sd: 0.073**

LogPcalc	LogPobs
1.856	1.829

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	0.455	0.003
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	3.816	0.001

											logL(calc)	logL(calc)	logL(obs)	
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	5.021	5.021	5.031	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.858	3.858	3.816	0.002
JCA (2000) 905 23	CP-SIL-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL-8CB	9.967	9.967	10.020	0.003
JAFC (2002) 50(8) 2385-2391		0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100		9.803	9.803	9.730	0.005
JAFC (2001) 49(9) 4315-4323		1.473	0.000	0.746	0.957	0.265	1.829	0.000	RI/100		10.028	10.028	10.100	0.005
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	10.015	10.015	10.080	0.004
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	9.679	9.679	9.730	0.003
JAFC (1984) 32(5) 1013		0.601	-0.257	0.942	1.309	0.000	1.996	0.000	RI/100		9.654	9.654	9.690	0.001
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	13.917	13.917	13.810	0.011
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	9.897	9.897	9.780	0.014