SMILES	CCc1nc(CC)cnc1			C_w=	
Compound No.	19911			C_g=	
Compound Name	**2,6-diethylpyrazine**			**log Kw=**	
Molecular Formula	C8H12N2			P + L, count:	11
Molecular weight	136.1944	**WS (mg/L)=**			
CAS No	13067-27-1	**VP (mm Hg)=**		**P+L, sd:**	**0.035**
ACD/n20 =	1.498				
E =	0.644			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.740		1.79	1.70	**P+L, sd(W):**	**0.035**

UNIX	**SMART**			**PA**		
0.73	0.623	logKw	3.624		P, count:	3
0.78		R (**E**)=	**0.623**	**0.67**		
0.00	0.00	Pi (**S**)=	0.670	**0.71**	**P, sd:**	**0.020**
0.58		Alpha (**A**) =	**0.000**	**0.00**		
4.98		Beta (**B**)=	0.740	**0.50**	L, count:	8
		LogL16 (**L**) =	4.724	**4.912**		
		Vx (**V**)=	1.1978		**L, sd:**	**0.041**

											LogPcalc	LogPobs		
											2.160	2.155		
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)	1.740	1.740	1.740	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.126	1.126	1.100	0.001	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.615	3.615	3.624	0.000	

											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	5.389	5.389	5.364	0.001
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.724	4.724	4.724	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.635	3.635	3.624	0.000
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	10.981	10.981	10.900	0.007
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	10.949	10.949	10.930	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	10.853	10.853	10.890	0.001
JAFC (2001) 49(9)	4315-4323	1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100		10.842	10.842	10.890	0.002
JAFC (2001) 49(3)	HP-Wax	-1.473	1.389	7.264	11.276	0.000	2.192	0.000	RI/100	HP-Wax	14.613	14.613	14.630	0.000