SMILES	Cc1cc[nH]c1	**OK**		**C_w=**	
Compound No.	19504			**C_g=**	
Compound Name	**3-Methylpyrrole**			**log Kw=**	
Molecular Formula	C5H7N			P + L, count:	7
Molecular weight	81.1200	**WS (mg/L)=**			
CAS No	616-43-3	**VP (mm Hg)=**		**P+L, sd:**	**0.049**
Beil/n20 =	1.497				
E =	**0.593**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.247	1.247	1.45	1.21	**P+L, sd(W):**	**0.049**

Pyrrole	**UNIX**	**SMART**					
			logKw	3.321	**PA**	P, count:	2
0.613	0.60		R (**E**)=	**0.593**	**0.53**		
0.910	0.68		Pi (**S**)=	0.900	**0.72**	**P, sd:**	**0.034**
0.220	0.37		Alpha (**A**) =	**0.240**	**0.31**		
0.250	0.43		Beta (**B**)=	0.290	**0.27**	L, count:	5
2.792	3.72		LogL16 (**L**) =	3.340	**3.593**		
			Vx (**V**)=	0.7183		**L, sd:**	**0.057**

LogPcalc	LogPobs
2.277	2.284

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)	1.217	1.217	1.247	0.001	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.337	3.337	3.321	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	4.566	4.566	4.568	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.307	3.307	3.321	0.000	
JAFC (2001) 49(9)	4315-4323	1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100		8.546	8.546	8.560	0.000	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	8.546	8.546	8.620	0.005	
JAFC (2002) 50(5)	BPX-5	0.411	0.000	1.247	1.297	0.169	2.033	0.000	RI/100	BPX-5	8.684	8.684	8.600	0.007	