SMILES	Cc1cccnH1	OK		C_w=	
Compound No.	19503			C_g=	
Compound Name	**2-Methylpyrrole**			**log Kw=**	
Molecular Formula	C5H7N			P + L, count:	10
Molecular weight	81.1200	**WS (mg/L)=**			
CAS No	636-41-9	**VP (mm Hg)=**		**P+L, sd:**	**0.039**
Beil/n20 =	1.502				
E =	**0.611**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.247	1.247	1.45	1.21	**P+L, sd(W):**	**0.039**

UNIX	**SMART**			**PA**		
		logKw	3.335		P, count:	2
0.60		R (**E**)=	**0.611**	0.53		
0.68		Pi (**S**)=	0.940	0.72	**P, sd:**	**0.019**
0.37		Alpha (**A**) =	0.240	0.31		
0.43		Beta (**B**)=	0.270	0.27	L, count:	8
3.72		LogL16 (**L**) =	3.336	3.593		
		Vx (**V**)=	0.7183		**L, sd:**	**0.043**

LogPcalc	LogPobs
2.303	2.291

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)	1.254	1.254	1.247	0.000	ClogP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.353	3.353	3.335	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	4.562	4.562	4.582	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.336	3.336	3.335	0.000
JAFC (2002) 50(5)	BPX-5	0.411	0.000	1.247	1.297	0.169	2.033	0.000	RI/100	BPX-5	8.722	8.722	8.660	0.004
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	8.454	8.454	8.500	0.002
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	8.575	8.575	8.560	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	8.486	8.486	8.550	0.004
Thesis German	DB-1	0.592	0.000	0.627	1.106	0.000	2.018	0.000	RI/100	DB-1	8.178	8.178	8.130	0.002
Thesis German	DB-Wax	-0.742	1.264	6.296	9.865	0.000	2.155	0.000	RI/100	DB-Wax	15.505	15.505	15.510	0.000