SMILES	C(c1ccco1)n2cccc2			C_w=	
Compound No.	19520			C_g=	
Compound Name	**N-Furfurylpyrrole**			**log Kw=**	
Molecular Formula	C9H9NO			P + L, count:	13
Molecular weight	147.1700	**WS (mg/L)=**			
CAS No	1438-94-4	**VP (mm Hg)=**		**P+L, sd:**	**0.076**
S-A/n20 =	1.531				
E =	0.826			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	2.158		2.44	1.88	**P+L, sd(W):** **0.076**

UNIX	**SMART**			**PA**		
0.96		logKw	3.466		P, count:	3
1.00		R (**E**)=	**0.826**	**0.87**		
0.00		Pi (**S**)=	1.100	**1.04**	**P, sd:**	**0.083**
0.59		Alpha (**A**) =	**0.000**	**0.00**		
5.38		Beta (**B**)=	0.460	**0.37**	L, count:	10
		LogL16 (**L**) =	5.061	**5.291**		
		Vx (**V**)=	1.1460		**L, sd:**	**0.079**

LogPcalc	LogPobs
2.463	2.406

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)	2.173	2.173	2.158	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	1.701	1.701	1.595	0.011	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.517	3.517	3.466	0.003	

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	5.583	5.583	5.624	0.002	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	5.061	5.061	5.061	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.561	3.561	3.466	0.009	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	12.014	na		na	11.820
JAFC (2001) 49(4)	BPX-5	0.553	0.000	0.976	1.078	0.345	1.988	0.000	RI/100	BPX-5	11.846	11.846	11.950	0.011	
Thesis German	DB-1	0.592	0.000	0.627	1.106	0.000	2.018	0.000	RI/100	DB-1	11.494	11.494	11.510	0.000	
Thesis German	DB-Wax	-0.742	1.264	6.296	9.865	0.000	2.155	0.000	RI/100	DB-Wax	18.134	18.134	18.200	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	11.591	na		na	11.330
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	11.609	11.609	11.480	0.017	
JAFC (2002) 50(8)	2385-2391	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100		11.638	11.638	11.660	0.001	
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	12.048	12.048	11.960	0.008	
JAFC (2001) 49(5)	BPX-5	0.531	0.000	1.112	1.077	0.000	2.037	0.000	RI/100	BPX-5	12.063	12.063	11.990	0.005	