SMILES	O=Cc1cccn1			C_w=	
Compound No.	**19529**			C_g=	
Compound Name	**2-Pyrrolecarbaldehyde**			**log Kw=**	
Molecular Formula	C5H5NO			P + L, count:	12
Molecular weight	95.1000	**WS (mg/L)=**			
CAS No	1003-29-8	**VP (mm Hg)=**		**P+L, sd:**	**0.073**
ACD/n20 =	1.607				
E =	0.982			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
0.640	0.210		0.74	0.64	**P+L, sd(W):**	**0.073**

UNIX	**SMART**			**PA**		
		logKw	4.840		P, count:	3
0.73		R (**E**)=	0.733	**0.76**		
1.17		Pi (**S**)=	1.390	**1.27**	**P, sd:**	**0.022**
0.37		Alpha (**A**) =	0.230	**0.31**		
0.77		Beta (**B**)=	0.340	**0.56**	L, count:	9
4.36		LogL16 (**L**) =	3.939	**4.434**		
		Vx (**V**)=	0.7340		**L, sd:**	**0.085**

	LogPcalc	LogPobs
	1.541	1.526

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)	0.666	0.666	0.640	0.001	**P***
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.899	-0.899	-0.901	0.000	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.857	4.857	4.840	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	5.464	5.464	5.480	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.939	3.939	3.939	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.840	4.840	4.840	0.000	
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	10.095	10.095	9.970	0.016	
JAFC (1976) 24(2)	OV-1	0.422	0.000	0.672	1.155	0.000	2.067	0.000	RI/100	OV-1	9.764	na		na	10.230
JAFC (2002) 50(8)	CP-Sil-5CB	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100	CP-Sil-5CB	9.669	9.669	9.860	0.036	
JAFC (1998) 2260-2265		1.589	0.000	0.742	0.824	0.000	1.744	0.000			9.680	9.680	9.640	0.002	
Z. Lebensm Unters	CW-20M	-0.666	0.000	6.634	9.895	0.000	2.199	0.000	RI/100	CW-20M	19.493	19.493	19.500	0.000	
Z. Lebensm Unters	Triton X-305	1.616	0.000	4.889	8.432	-1.533	1.906	0.000	RI/100	Triton X-305	17.338	17.338	17.350	0.000	
Z. Lebensm Unters	DB-5	0.489	-0.409	1.331	1.041	0.000	2.055	0.000	RI/100	DB-5	10.374	10.374	10.310	0.004	