SMILES	c1(nccc1)C(C)=O				C_w=	
Compound No.	19527				C_g=	
Compound Name	**2-Acetylpyrrole**	**Trivial alteration**			**log Kw=**	
Molecular Formula	C6H7NO				P + L, count:	14
Molecular weight	109.1300	**WS (mg/L)=**				
CAS No	1072-83-9	**/P (mm Hg)=**			**P+L, sd:**	**0.059**
ACD/n20 =	1.530					
E =	0.750				Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
0.930	0.595	0.595	0.89	0.88	**P+L, sd(W):**	**0.059**

0.057							
5.425	**UNIX**	**SMART**	logKw	5.415	PA	P, count:	2
0.809	0.74		R (**E**)=	0.750	**0.74**		
1.010	1.15		Pi (**S**)=	1.000	**1.22**	**P, sd:**	**0.027**
0.390	0.37		Alpha (**A**) =	0.400	**0.31**		
0.550	0.77		Beta (**B**)=	0.550	**0.58**	L, count:	12
4.271	4.84		LogL16 (**L**) =	4.271	**4.793**		
0.8749			Vx (**V**)=	0.8749		**L, sd:**	**0.063**

											LogPcalc	LogPobs		
											3.159	3.172		
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)	0.903	0.903	0.930	0.001	P*
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.415	5.415	5.415	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	6.371	6.371	6.345	0.001	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.388	5.388	5.415	0.001	
JCA (2000) 905 23	CP-SIL-8CB	0.469	-0.215	1.298	1.001	0.000	2.032	0.000	RI/100	CP-SIL-8CB	10.686	10.686	10.680	0.000	
JAFC (2000) 48(6)	DB-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	DB-5	10.745	10.745	10.630	0.013	
JAFC (2002) 50(8)	2385-2391	0.604	0.000	0.599	0.685	0.000	2.050	0.000	RI/100		10.233	10.233	10.300	0.004	
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	19.531	na		na	19.100
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	10.544	10.544	10.640	0.009	
JAFC (1994) 42(3)	DB-1	0.497	0.000	0.738	0.967	0.000	2.018	0.000	RI/100	DB-1	10.241	10.241	10.240	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	10.692	na		na	10.240
JAFC (2001) 49(5)	BPX-5	0.531	0.000	1.112	1.077	0.000	2.037	0.000	RI/100	BPX-5	10.775	10.775	10.860	0.007	
JAFC (1989) 37(3)	Basic	0.306	0.000	0.789	0.918	0.000	2.069	0.000	RI/100	Basic	10.300	10.300	10.210	0.008	
JAFC (1989) 37(3)	Acidic	0.236	0.720	0.546	0.881	0.342	1.962	0.000	RI/100	Acidic	10.243	10.243	10.230	0.000	
Thesis German	DB-1	0.592	0.000	0.627	1.106	0.000	2.018	0.000	RI/100	DB-1	10.281	10.281	10.260	0.000	
Thesis German	DB-Wax	-0.742	1.364	6.296	9.865	0.000	2.155	0.000	RI/100	DB-Wax	19.728	19.728	19.740	0.000	
Qual Anal Flav Fra	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	10.774	na		na	10.500
Qual Anal Flav Fra	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	18.741	na		na	19.350