SMILES	O=C(C)OCc1occc1				
Compund No.	18529				
Compund Name	**Furfuryl acetate**				
Molecular Formula	C7H8O3			P + L, count:	10
Molecular weight	140.1366				
CAS No	623-17-6			**P+L, sd:**	**0.082**
S-A/n20 =	1.462				
E =	**0.440**			Weight:	1.00
ClogP	**ClogP(MD)**	**ClogP(PA)**	**ClogP(ACD)**		
1.136	1.136	1.09	1.09	**P+L, sd(W):**	**0.082**

UNIX	**SMART**			**PA**		
		logKw	3.742		P, count:	2
0.55	0.439	R (**E**)=	**0.440**	**0.50**		
0.89	0.95	Pi (**S**)=	1.010	**0.95**	**P, sd:**	**0.069**
0.00	0.00	Alpha (**A**) =	**0.000**	**0.02**		
0.51	0.55	Beta (**B**)=	0.580	**0.56**	L, count:	8
4.12	4.139	LogL16 (**L**) =	4.056	**4.152**		
		Vx (**V**)=	**1.0334**		**L, sd:**	**0.089**

											LogPcalc	LogPobs		
											2.475	2.439		
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)	1.205	1.205	1.136	0.005	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.744	3.744	3.742	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	4.828	4.828	4.878	0.002	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.789	3.789	3.742	0.002	
JAFC (2001) 49(3) 1345-1352		0.782	-0.451	1.312	0.808	0.000	1.975	0.000	RI/100		9.920	9.920	9.910	0.000	
JAFC (1981) 29(1)	CW-20W	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20W	15.112	15.112	15.140	0.001	
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	9.656	9.656	9.670	0.000	
"Qualitative Analy	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	9.876	9.876	9.690	0.034	
"Qualitative Analy	CW-20W	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20W	14.747	na		na	
JAFC (1989) 37(3) 814-819 Basic		0.306	0.000	0.789	0.918	0.000	2.069	0.000	RI/100		9.495	9.495	9.620	0.016	
JAFC (1989) 37(3) 814-819 Acidic		0.236	0.720	0.546	0.881	0.342	1.962	0.000	RI/100		9.261	na		na	
Meat Sci (1996) 44	DB-5	0.493	-0.430	1.327	1.408	0.000	2.048	0.000	RI/100	DB-5	9.951	9.951	9.950	0.000	