SMILES	O(C(=O)c1ccco1)C			C_w=	
Compound No.	18539			C_g=	
Compound Name	**Methyl 2-furoate**			**log Kw=**	
Molecular Formula	C6H6O3			P + L, count:	12
Molecular weight	126.1100	**WS (mg/L)=**			
CAS No	611-13-2	**VP (mm Hg)=**		**P+L, sd:**	**0.075**
S-A/n20 =	1.487				
E =	**0.565**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
1.000	1.290	1.287	1.11	0.99	**P+L, sd(W):**	**0.075**

UNIX	**SMART**			**PA**		
		logKw	3.647		P, count:	3
0.55	0.560	R (**E**)=	**0.565**	0.43		
0.89	1.00	Pi (**S**)=	1.110	0.91	**P, sd:**	**0.026**
0.00	0.00	Alpha (**A**) =	0.000	0.00		
0.51	0.50	Beta (**B**)=	0.470	0.48	L, count:	9
3.62		LogL16 (**L**) =	3.952	3.617		
		Vx (**V**)=	**0.8925**		**L, sd:**	**0.087**

LogPcalc	LogPobs
1.670	1.651

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)	1.013	1.013	1.000	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	0.337	0.337	0.305	0.001
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	3.661	3.661	3.647	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	4.653	4.653	4.647	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.952	3.952	3.952	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	3.659	3.659	3.647	0.000
Flav Frag J (2003)	SPB-5	0.675	-0.682	1.434	1.276	-0.312	2.044	0.000	RI/100	SPB-5	9.814	9.814	9.800	0.000
Flav Frag J (2002)	SPB-5	0.552	-0.435	1.225	1.251	0.000	2.049	0.000	RI/100	SPB-5	9.764	9.764	9.830	0.004
Flav Frag J (2003)	AT-Wax	-0.913	0.945	6.681	10.737	0.000	2.214	0.000	RI/100	AT-Wax	15.787	15.787	15.630	0.025
Flav Frag J (2003)	CP-SIL-5CB	0.347	-0.592	1.179	1.113	-0.341	2.092	0.000	RI/100	CP-SIL-5CB	9.429	9.429	9.370	0.004
Anal Chem (1993)	OV-101	0.426	-0.311	1.145	1.189	0.000	2.034	0.000	RI/100	OV-101	9.560	9.560	9.560	0.000
Anal Chem (1993)	CW-20M	0.249	1.200	6.184	8.439	-0.765	2.027	0.000	RI/100	CW-20M	15.443	15.443	15.610	0.028