SMILES	C(O)c1oc(cc1)C=O			C_w=	
Compound No.	18548			C_g=	
Compound Name	**5-Hydroxymethyl-2-furaldehyde**			**log Kw=**	
Molecular Formula	C6H6O3			P + L, count:	8
Molecular weight	126.1100	**WS (mg/L)=**			
CAS No	67-47-0	**VP (mm Hg)=**		**P+L, sd:**	**0.074**
S-A/n20 =	1.562				
E =	**0.892**			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	-0.367	-0.367	-0.34	-0.45	**P+L, sd(W):**	**0.074**

A = 0.65							
8.639	**UNIX**	**SMART**	logKw	8.039	**PA**	P, count:	2
0.892	0.81		R (**E**)=	**0.892**	**0.84**		
1.120	1.23		Pi (**S**)=	1.450	**1.21**	**P, sd:**	**0.105**
0.650	0.35		Alpha (**A**) =	0.400	**0.31**		
0.940	0.93		Beta (**B**)=	0.850	**0.85**	L, count:	6
4.797	4.35		LogL16 (**L**) =	4.838	**4.673**		
0.8925			Vx (**V**)=	0.8925		**L, sd:**	**0.074**

LogPcalc	LogPobs
3.810	3.836

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)	-0.463	-0.463	-0.367	0.009	MedChem
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	8.082	8.082	8.039	0.002	

											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	7.605	7.605	7.672	0.004	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	8.063	8.063	8.039	0.001	
JAFC (1998) 46(2)	CP-Sil-5CB	0.572	0.000	1.006	1.348	-0.654	2.024	0.000	RI/100	CP-Sil-5CB	11.807	11.807	11.730	0.006	
Food Chem (1999)	CP-Sil-5CB	0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100	CP-Sil-5CB	12.082	na		na	11.750
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	23.806	23.806	23.920	0.013	
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	12.068	na		na	12.670
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	12.251	na		na	11.600
JAFC (1998) 46(6)	DB-1	1.589	0.000	0.742	0.824	0.000	1.744	0.000	RI/100	DB-1	11.432	na		na	11.950
JAFC (2000) 48(6)	DB-1	0.643	0.000	0.730	0.903	0.000	2.007	0.000	RI/100	DB-1	11.773	11.773	11.760	0.000	
Z Lebensm Unters	CW-20M	-0.666	0.000	6.634	9.895	0.000	2.199	0.000	RI/100	CW-20M	23.552	na		na	24.100
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	19.998	na		na	21.350
J Nat Med (2006) 6	DB-5MS	0.598	-0.858	1.687	1.566	0.000	1.991	0.000	RI/100	DB-5MS	12.538	na		na	12.260
J Nat Med (2006) 6	TC-Wax	-1.343	0.000	8.016	10.875	0.000	2.146	0.000	RI/100	TC-Wax	25.015	25.015	24.960	0.003	