SMILES	c1(oc(cc1)C)C=O		C_w=	
Compound No.	18534		C_g=	
Compound Name	**5-Methylfurfural**		**log Kw=**	
Molecular Formula	C6H6O2		P + L, count:	43
Molecular weight	110.1100	**WS (mg/L)=**		
CAS No	620-02-0	**VP (mm Hg)=**	**P+L, sd:**	**0.063**
S-A/n20 =	1.531			
E =	**0.744**		Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	1.170		1.11	1.19	**P+L, sd(W):**	**0.063**

UNIX	**SMART**			**PA**		
0.65	0.744	logKw	4.028		P, count:	13
0.93	1.16	R (**E**)=	**0.744**	**0.62**		
0.00	0.00	Pi (**S**)=	1.110	**1.00**	**P, sd:**	**0.067**
0.50	0.51	Alpha (**A**) =	0.000	**0.00**		
3.65	4.013	Beta (**B**)=	0.520	**0.44**	L, count:	30
		LogL16 (**L**) =	3.933	**3.822**		
		Vx (**V**)=	0.8338		**L, sd:**	**0.062**

											LogPcalc	LogPobs	
											1.011	0.981	
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)	0.717	0.717	**0.670**	0.002
b	Pentanol	0.175	0.575	-0.787	0.020	-2.837	0.000	3.249	P	Pentanol	0.963	0.963	0.870	0.009
b	Decanol	0.008	0.485	-0.974	0.015	-3.798	0.000	3.945	P	Decanol	0.602	0.602	0.560	0.002
CTET-1	Tetrachloromethane	0.260	0.573	-1.254	-3.558	-4.588	0.000	4.589	P	CCl4 Sept 98	0.735	0.735	0.660	0.006
Caroline	Decane August 98	0.160	0.585	-1.734	-3.435	-5.078	0.000	4.582	P	Decane August 98	-0.150	-0.150	-0.150	0.000
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-0.047	-0.047	-0.095	0.002
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.057	4.057	4.028	0.001
BENZ-1	Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491	P	Benzene/Dec/1997 (25ce	1.174	1.174	1.100	0.005
BENZ-1	Toluene	0.143	0.527	-0.720	-3.010	-4.824	0.000	4.545	P	Toluene/Dec/1997	1.017	1.017	0.980	0.001
PHCL-1	Chlorobenzene	0.040	0.246	-0.462	-3.038	-4.769	0.000	4.640	P	Chlorobenzene	1.099	1.099	1.210	0.012
AMAL	Bromobenzene	-0.130	0.394	-0.280	-3.331	-4.640	0.000	4.583	P	Bromobenzene	1.261	1.261	1.200	0.004
AMAL	Iodobenzene	-0.181	0.410	-0.334	-3.300	-4.595	0.000	4.549	P	Iodobenzene	1.157	1.157	1.090	0.004
AMAL	Diisopropylether	0.476	0.434	-0.939	-0.555	-5.185	0.000	4.189	P	Diisopropyl ether/ Wet/ 2(	0.553	0.553	0.630	0.006

											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	4.708	4.708	4.698	0.000
CTET-1	Tetrachloromethane	0.282	-0.303	0.460	0.000	0.000	1.047	0.000	L	CCl4/Sept 98	4.685	4.685	4.688	0.000
Caroline	Decane	0.156	-0.143	0.000	0.000	0.000	0.989	0.000	L	Decane	3.939	3.939	3.878	0.004

	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	3.933	3.933	3.933	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.051	4.051	4.028	0.001	
BENZ-1	Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000	L	Benzene/Dec 97	5.142	5.142	5.128	0.000	
BENZ-1	Toluene	0.121	-0.222	0.938	0.467	0.099	1.012	0.000	L	Toluene/Dec 97	5.029	5.029	5.008	0.000	
PHCL-1	Chlorobenzene	0.053	-0.553	1.254	0.364	0.000	1.041	0.000	L	Chlorobenzene	5.128	5.128	5.238	0.012	
"Qualit Anal Flav F	OV-101	0.538	0.224	1.011	1.009	0.000	2.026	0.000	RI/100	OV-101	9.795	na		na	9.420
"Qualit Anal Flav F	CW-20M	0.226	1.469	5.468	7.877	0.000	2.059	0.000	RI/100	CW-20M	15.486	15.486	15.630	0.021	
JSFA (2003) 83 275-282		-0.808	1.272	6.138	9.312	0.000	2.160	0.000	RI/100		15.447	15.447	15.400	0.002	
Meat Sci (1996) 44(4) 255-273		0.493	-0.430	1.327	1.408	0.000	2.048	0.000	RI/100		9.701	9.701	9.710	0.000	
JAFC (1998) 46(4)	BPX-5	0.348	0.000	1.031	0.889	0.261	2.064	0.000	RI/100	BPX-5	9.746	9.746	9.770	0.001	
JAFC (2000) 48(8)	BPX-5	0.616	0.000	1.052	0.947	0.226	2.003	0.000	RI/100	BPX-5	9.779	9.779	9.780	0.000	
JAFC (1985) 33(2)	DB-1	0.536	-0.429	1.171	1.260	-0.229	2.016	0.000	RI/100	DB-1	9.326	9.326	9.260	0.004	
JAFC (1991) 39(11	DB-Wax	0.465	-1.373	4.806	1.418	-4.049	2.009	0.000	RI/100	DB-Wax	10.574	na		na	9.650
JAFC (1993) 41(11) 2056-2062		0.504	0.000	0.458	0.000	0.885	2.003	0.000	RI/100		9.350	9.350	9.290	0.004	
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	9.742	9.742	9.670	0.005	
JAFC (2001) 49(9) 4315-4323		1.344	0.000	0.769	0.978	0.330	1.850	0.000	RI/100		9.645	9.645	9.800	0.024	
JAFC (2002) 50(21	CP-SIL-5CB	0.194	-0.505	0.955	0.886	0.000	2.119	0.000	RI/100	CP-SIL-5CB	9.212	9.212	9.240	0.001	
JAFC (2002) 50(21	AT-Wax	-0.807	1.004	6.501	10.459	0.000	2.151	0.000	RI/100	AT-Wax	15.616	15.616	15.560	0.003	
Flav Frag J. (2003)	SPB-5	0.675	-0.682	1.434	1.276	-0.312	2.044	0.000	RI/100	SPB-5	9.636	9.636	9.630	0.000	
JAFC (1989) 37(3)	Basic	0.306	0.000	0.789	0.918	0.000	2.069	0.000	RI/100	Basic	9.319	9.319	9.260	0.003	
JAFC (1989) 37(3)	Acid	0.236	0.720	0.546	0.881	0.342	1.962	0.000	RI/100	Acid	9.272	9.272	9.260	0.000	
JAFC (1981) 29(1)	CW-20M	-0.359	0.703	6.654	9.550	0.000	2.081	0.000	RI/100	CW-20M	15.734	na		na	15.440
JAFC (1981) 29(1)	OV-101	0.439	0.000	0.764	1.121	0.000	2.082	0.000	RI/100	OV-101	9.475	na		na	9.870
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	9.373	9.373	9.270	0.011	
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	9.254	9.254	9.310	0.003	
JAFC (1998) 46(2)	HP-Wax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	HP-Wax	15.356	na		na	15.580
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	9.309	9.309	9.350	0.002	
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	9.878	9.878	9.820	0.003	
JAFC (1999) 47(4)	BPX-5	0.917	0.000	0.995	1.089	0.310	1.938	0.000	RI/100	BPX-5	9.805	9.805	9.790	0.000	
JAFC (1999) 47(12	CPWax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CPWax-52CB	15.295	na		na	15.630
JAFC (1999) 47(12	CP-SIL-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CP-SIL-8CB	9.552	9.552	9.580	0.001	
JAFC (2002) 50(7) 2010-2015		0.138	0.965	5.980	8.691	0.000	2.089	0.000	RI/100		15.710	na		na	15.180
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	9.331	9.331	9.310	0.000	
Food Chem. (1999) 64 3-11		0.045	-0.609	1.664	1.596	-0.555	2.067	0.000	RI/100		9.280	9.280	9.350	0.005	