SMILES	C=1C(\C(=C(/OC=1)C)O)=O			C_w=	
Compound No.	18624			C_g=	
Compound Name	**Maltol**			**log Kw=**	
Molecular Formula	C6H6O3			P + L, count:	11
Molecular weight	126.1100	**WS (mg/L)=**			
CAS No	118-71-8	**VP (mm Hg)=**		**P+L, sd:**	**0.076**
ACD/n20 =	1.560				
E =	0.884			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
0.020	0.020	0.100	0.15	0.08	**P+L, sd(W):**	**0.076**

with E = 1.00							
6.333	**UNIX**	**SMART**	logKw	6.332	**PA**	P, count:	3
1.003	0.82		R (**E**)=	0.930	**0.93**		
1.190	1.23		Pi (**S**)=	1.180	**1.28**	**P, sd:**	**0.073**
0.150	0.55		Alpha (**A**) =	0.160	**0.31**		
0.810	0.80		Beta (**B**)=	0.810	**0.97**	L, count:	8
4.672	4.47		LogL16 (**L**) =	4.658	**4.652**		
0.8925			Vx (**V**)=	0.8925		**L, sd:**	**0.082**

LogPcalc	LogPobs
1.506	1.559

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)	-0.026	-0.026	0.020	0.002	P*
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	-1.762	-1.762	-1.673	0.008	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	6.306	6.306	6.332	0.001	

Ref	Solvent	c	e	s	a	b	l	v	P or L?	Solvent	logL(calc)	logL(calc)	logL(obs)	(Po-Pc)^2	
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	6.358	6.358	6.352	0.000	
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	4.658	4.658	4.658	0.000	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	6.262	6.262	6.332	0.005	
JAFC (1991) 39(11	DB-5	0.465	-1.373	4.806	1.418	-4.049	2.009	0.000	RI/100	DB-5	11.165	11.165	11.120	0.002	
JAFC (1998) 46(2)	HP-1	0.477	-0.574	1.064	1.465	0.000	2.040	0.000	RI/100	HP-1	10.936	10.936	11.040	0.011	
JAFC (1998) 46(2)	Innowax	-0.707	0.931	5.690	10.871	1.090	2.158	0.000	RI/100	Innowax	19.548	19.548	19.540	0.000	
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	10.970	10.970	10.860	0.012	
JAFC (1997) 45(3)	DB-1	0.520	0.000	0.978	1.894	0.000	1.975	0.000	RI/100	DB-1	11.177	na		na	10.700
JAFC (1998)46(6)	DB-1	1.589	0.000	0.742	0.824	0.000	1.744	0.000	RI/100	DB-1	10.720	10.720	10.850	0.017	