SMILES	COc1cc(\C=C\C)ccc1O			C_w=	
Compound No.	16842			C_g=	
Compound Name	**Isoeugenol**			**log Kw=**	
Molecular Formula	C10H12O2			P + L, count:	21
Molecular weight	164.2000	**WS (mg/L)=**			
CAS No	97-54-1	**VP (mm Hg)=**		**P+L, sd:**	**0.072**
Beil/n20 =	1.571				
E =	**1.140**			Weight:	1.00
P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**	
	2.577	3.040	2.61	2.45	**P+L, sd(W):** **0.072**

UNIX	**SMART**			**PA**		
		logKw	4.643		P, count:	9
1.03	0.950	R (**E**)=	**1.140**	**0.94**		
0.84	1.05	Pi (**S**)=	0.950	**1.01**	**P, sd:**	**0.065**
0.29	0.22	Alpha (**A**) =	0.310	**0.27**		
0.62	0.64	Beta (**B**)=	0.540	**0.54**	L, count:	12
5.93	6.165	LogL16 (**L**) =	6.286	**6.000**		
		Vx (**V**)=	1.3544		**L, sd:**	**0.079**

LogPcalc	LogPobs
2.144	2.118

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)	3.035	3.035	3.040	0.000	MD
Caroline	Pentane August 98	0.369	0.386	-1.568	-3.535	-5.215	0.000	4.514	P	Pentane August 98	1.521	1.521	1.580	0.003	
Caroline	Hexane August 98	0.361	0.579	-1.723	-3.599	-4.764	0.000	4.344	P	Hexane August 98	1.579	1.579	1.540	0.002	
Caroline	Heptane August 98	0.325	0.670	-2.061	-3.317	-4.733	0.000	4.543	P	Heptane August 98	1.700	1.700	1.630	0.005	
Caroline	Octane August 98	0.223	0.642	-1.647	-3.480	-5.067	0.000	4.526	P	Octane August 98	1.705	1.705	1.640	0.004	
Caroline	Nonane August 98	0.240	0.619	-1.713	-3.532	-4.921	0.000	4.482	P	Nonane August 98	1.636	1.636	1.620	0.000	
Caroline	Decane August 98	0.160	0.585	-1.734	-3.435	-5.078	0.000	4.582	P	Decane August 98	1.578	1.578	1.640	0.004	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.705	4.705	4.643	0.004	
CYC-1	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	P	Cyclohexane/Dec 98	1.837	1.837	1.730	0.011	

											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	7.733	7.733	7.683	0.003	
Caroline	Pentane	0.335	-0.276	0.000	0.000	0.000	0.968	0.000	L	Pentane	6.105	6.105	6.223	0.014	
Caroline	Hexane	0.292	-0.169	0.000	0.000	0.000	0.979	0.000	L	Hexane	6.253	6.253	6.183	0.005	
Caroline	Heptane	0.275	-0.162	0.000	0.000	0.000	0.983	0.000	L	Heptane	6.269	6.269	6.273	0.000	
Caroline	Octane	0.215	-0.049	0.000	0.000	0.000	0.967	0.000	L	Octane	6.237	6.237	6.283	0.002	
Caroline	Nonane	0.200	-0.145	0.000	0.000	0.000	0.980	0.000	L	Nonane	6.195	6.195	6.263	0.005	
Caroline	Decane	0.156	-0.143	0.000	0.000	0.000	0.989	0.000	L	Decane	6.209	6.209	6.283	0.005	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.743	4.743	4.643	0.010	
CYC-1	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013	0.000	L	Cyclohexane/Dec/98	6.405	6.405	6.373	0.001	
JAFC (2000) 48(2)	DB-Wax	-1.307	0.523	9.055	10.206	0.000	1.977	0.000	RI/100	DB-Wax	23.482	23.482	23.520	0.001	
JAFC (2000) 48(2)	DB-5	-0.139	-1.242	2.721	2.102	0.000	2.016	0.000	RI/100	DB-5	14.353	14.353	14.380	0.001	
JAFC (2000) 48(6)	DB-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	DB-5	14.599	14.599	14.450	0.022	
Flav Frag J (2000)	Thermon 600T	0.282	1.113	5.971	9.485	0.000	2.041	0.000	RI/100	Thermon 600T	22.993	na		na	22.550
Flav Frag J (2000)	DB-5	0.686	-0.354	1.461	1.410	-0.370	2.004	0.000	RI/100	DB-5	14.504	na		na	13.970