SMILES	COc1c2c(cc(c1)CC=C)OCO2			C_w=	
Compound No.	**18743**			C_g=	
Compound Name	**Myristicin**			**log Kw=**	
Molecular Formula	C11H12O3			P + L, count:	12
Molecular weight	192.2100	**WS (mg/L)=**			
CAS No	607-91-0	**VP (mm Hg)=**		**P+L, sd:**	**0.056**
ACD/n20 =	1.539				
E =	0.960			Weight:	1.00

P*	**ClogP**	**logP(MD)**	**logP(PA)**	**logP(ACD)**		
	2.765	3.172	3.17	3.26	**P+L, sd(W):**	**0.056**

UNIX	**SMART**			**PA**		
1.17		logKw	4.584		P, count:	3
1.11		R (**E**)=	1.162	**1.08**		
0.00		Pi (**S**)=	1.230	**1.47**	**P, sd:**	**0.063**
1.04		Alpha (**A**) =	0.000	**0.00**		
6.48		Beta (**B**)=	0.630	**0.76**	L, count:	9
		LogL16 (**L**) =	6.712	**7.057**		
		Vx (**V**)=	1.4454		**L, sd:**	**0.058**

LogPcalc	LogPobs
3.199	3.159

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)	2.778	2.778	2.765	0.000	ClogP
	Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433	P	Hexadecane LogP16	2.213	2.213	2.128	0.007	
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.606	4.606	4.584	0.000	

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	7.336	7.336	7.349	0.000
	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000	0.000	L	Hexadecane	6.712	6.712	6.712	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.661	4.661	4.584	0.006
JCA (2002) 976 26	FSOT RSL-200	0.708	0.000	0.803	1.621	0.000	1.978	0.000	RI/100	FSOT RSL-200	14.972	14.972	15.020	0.002
JAFC (1999) 47(12	CP-Wax-52CB	-0.451	1.122	5.855	9.998	0.000	2.139	0.000	RI/100	CP-Wax-52CB	22.412	22.412	22.470	0.003
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	15.216	15.216	15.220	0.000
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	15.398	15.398	15.280	0.014
JAFC (1997) 45(7)	BPX-5	0.498	0.000	1.157	0.000	0.000	2.052	0.000	RI/100	BPX-5	15.694	15.694	15.660	0.001
JAFC (1996) 44(3)	DB-1	0.610	-0.430	1.328	1.728	-0.541	2.004	0.000	RI/100	DB-1	14.854	14.854	14.840	0.000