SMILES	c1(ccc(c(c1)OC)O)C
Compund No.	16837
Compund Name	**2-Methoxy-4-methylphenol**
Molecular Formula	C8H10O2
Molecular weight	138.1638
CAS No	93-51-6
S-A/n20 =	1.537
E =	**0.850**

P + L, count:	9
P+L, sd:	**0.054**
Weight:	1.00
P+L, sd(W):	**0.054**

ClogP	**ClogP(MD)**	**ClogP(PA)**	**ClogP(ACD)**
1.823	1.823	1.85	1.82

UNIX	**SMART**			**PA**		
0.89	0.850	logKw	4.924		P, count:	2
0.74	0.91	R (**E**)=	**0.850**	**0.83**		
0.29	0.15	Pi (**S**)=	0.840	**0.99**	**P, sd:**	**0.015**
0.60	0.59	Alpha (**A**) =	0.340	**0.36**		
4.99	4.990	Beta (**B**)=	0.610	**0.47**	L, count:	7
		LogL16 (**L**) =	4.982	**5.136**		
		Vx (**V**)=	**1.1156**		**L, sd:**	**0.062**

LogPcalc	LogPobs
3.377	3.373

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)	1.836	1.836	1.823	0.000	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	4.918	4.918	4.924	0.000	

											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	6.742	6.742	6.747	0.000
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	4.935	4.935	4.924	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	19.477	19.477	19.450	0.001
JAFC (1999) 47(12	CPSil-8CB	0.527	-0.150	1.099	1.329	0.000	2.013	0.000	RI/100	CPSil-8CB	11.804	11.804	11.870	0.004
JAFC (2000) 48(6)	DB-5	0.307	-0.424	1.298	1.348	0.000	2.088	0.000	RI/100	DB-5	11.898	11.898	11.900	0.000
Flav Frag J. (1999) 14 303-311		0.235	-0.456	1.246	1.000	0.000	2.097	0.000	RI/100		11.682	11.682	11.570	0.012
Food Res Int (2001	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	11.848	11.848	11.920	0.005

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