SMILES	c1cc(ccc1O)C=C
Compund No.	16584
Compund Name	**4-Vinylphenol**
Molecular Formula	C8H8O
Molecular weight	120.1485
CAS No	2628-17-3
ACD/n20 =	1.602
E =	**1.132**

	P + L, count:	9
	P+L, sd:	**0.082**
	Weight:	1.00
	P+L, sd(W):	**0.082**
	P, count:	2
	P, sd:	**0.055**
	L, count:	7
	L, sd:	**0.091**

	MD	**PA**	**ACD**
ClogP	2.199	2.25	2.16

UNIX	**SMART**			**PA**
1.07	1.044	logKw	5.398	
0.90	1.03	R (**E**)=	**1.044**	0.96
0.55	0.63	Pi (**S**)=	0.98	0.89
0.46	0.32	Alpha (**A**) =	**0.63**	0.60
4.63		Beta (**B**)=	0.37	0.34
		LogL16 (**L**) =	4.984	4.679
		Vx (**V**)=	**1.0139**	

LogPcalc	LogPobs
3.834	3.799

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)	2.250	2.250	2.199	0.003	CLOGP
d	Gas phase	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	P	Gas phase LogLW	5.419	5.419	5.398	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	7.521	7.521	7.597	0.006	
	Water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	L	Water	5.454	5.454	5.398	0.003	
JAFC (2001) 49(10	DB-Wax	-1.301	0.000	7.705	11.075	0.000	2.181	0.000	RI/100	DB-Wax	24.097	24.097	24.150	0.003	
JAFC (1998) 46(12	BPX-5	0.589	0.000	1.169	1.084	0.000	2.032	0.000	RI/100	BPX-5	12.545	12.545	12.470	0.006	
JAFC (1995) 43(7)	DB-1	0.313	0.000	0.637	0.865	0.241	2.058	0.000	RI/100	DB-1	11.828	11.828	11.900	0.005	
Food Chemistry (2003) 80 353-358		0.420	-0.340	0.893	0.779	0.000	2.054	0.000	RI/100		11.668	11.668	11.730	0.004	
Food Research Int.	DB-5	0.381	-0.568	1.700	1.392	-0.254	2.048	0.000	RI/100	DB-5	12.444	12.444	12.290	0.024	